



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 01:49 am BST

PDB ID : 1A5U  
Title : PYRUVATE KINASE COMPLEX WITH BIS MG-ATP-NA-OXALATE  
Authors : Larsen, T.M.; Benning, M.M.; Rayment, I.; Reed, G.H.  
Deposited on : 1998-02-18  
Resolution : 2.35 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

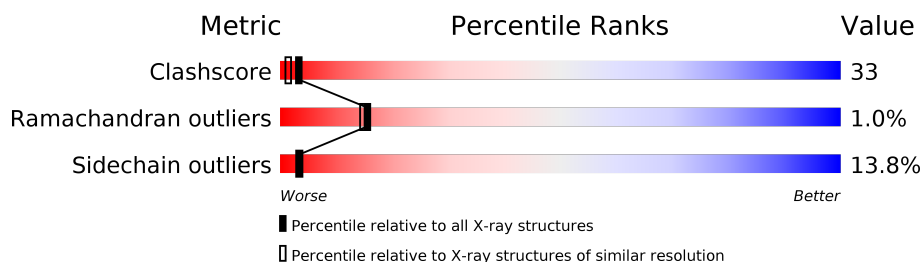
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	530	
1	B	530	
1	C	530	
1	D	530	
1	E	530	
1	F	530	
1	G	530	
1	H	530	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	OXL	A	533	-	-	X	-
3	OXL	F	4133	-	-	X	-
3	OXL	G	4733	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 33890 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called PYRUVATE KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	519	Total	C	N	O	S	0	0	0
			3978	2498	708	744	28			
1	B	519	Total	C	N	O	S	0	0	0
			3978	2498	708	744	28			
1	C	519	Total	C	N	O	S	0	0	0
			3978	2498	708	744	28			
1	D	519	Total	C	N	O	S	0	0	0
			3978	2498	708	744	28			
1	E	519	Total	C	N	O	S	0	0	0
			3978	2498	708	744	28			
1	F	519	Total	C	N	O	S	0	0	0
			3978	2498	708	744	28			
1	G	519	Total	C	N	O	S	0	0	0
			3978	2498	708	744	28			
1	H	519	Total	C	N	O	S	0	0	0
			3978	2498	708	744	28			

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

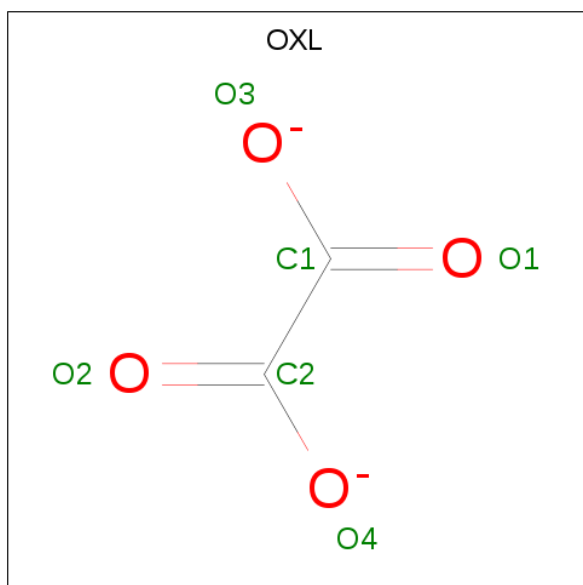
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Na	0	0
			1	1		
2	D	1	Total	Na	0	0
			1	1		
2	E	1	Total	Na	0	0
			1	1		
2	H	1	Total	Na	0	0
			1	1		
2	B	1	Total	Na	0	0
			1	1		
2	C	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		
2	F	1	Total	Na	0	0
			1	1		

- Molecule 3 is OXALATE ION (three-letter code: OXL) (formula:  $\text{C}_2\text{O}_4$ ).

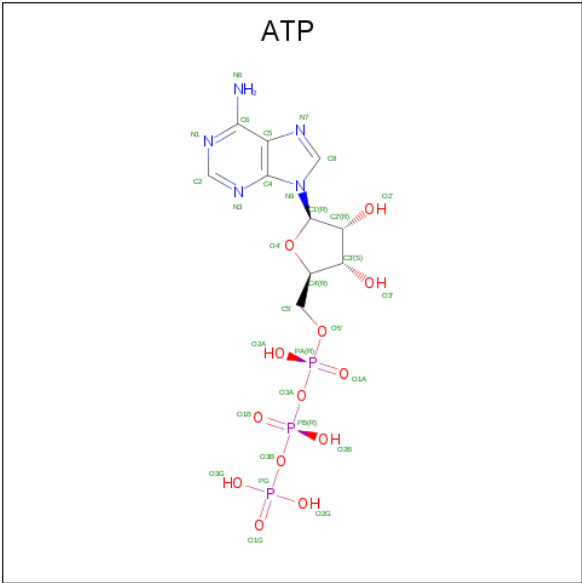


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	2	4		
3	B	1	Total	C	O	0	0
			6	2	4		
3	C	1	Total	C	O	0	0
			6	2	4		
3	D	1	Total	C	O	0	0
			6	2	4		
3	E	1	Total	C	O	0	0
			6	2	4		
3	F	1	Total	C	O	0	0
			6	2	4		
3	G	1	Total	C	O	0	0
			6	2	4		
3	H	1	Total	C	O	0	0
			6	2	4		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula:  $\text{Mg}$ ).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	2	Total	Mg	0	0
			2	2		
4	D	2	Total	Mg	0	0
			2	2		
4	E	2	Total	Mg	0	0
			2	2		
4	H	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		
4	C	2	Total	Mg	0	0
			2	2		
4	A	2	Total	Mg	0	0
			2	2		
4	F	2	Total	Mg	0	0
			2	2		

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
5	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
5	G	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 6 is water.

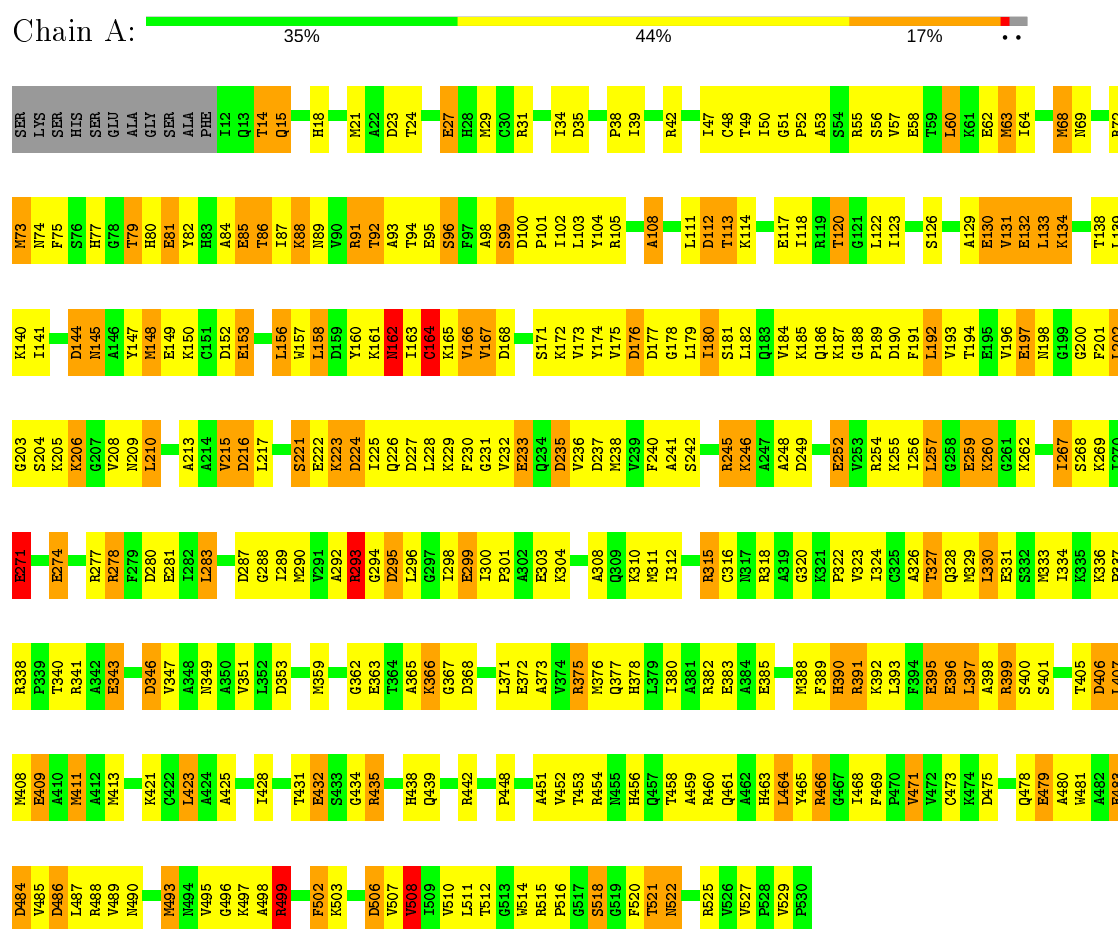
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	176	Total	O	0	0
			176	176		
6	B	260	Total	O	0	0
			260	260		
6	C	166	Total	O	0	0
			166	166		
6	D	250	Total	O	0	0
			250	250		
6	E	267	Total	O	0	0
			267	267		
6	F	185	Total	O	0	0
			185	185		
6	G	210	Total	O	0	0
			210	210		
6	H	296	Total	O	0	0
			296	296		

### 3 Residue-property plots

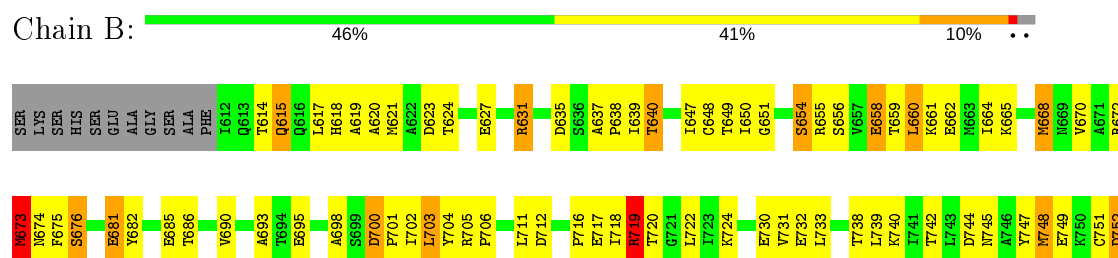
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

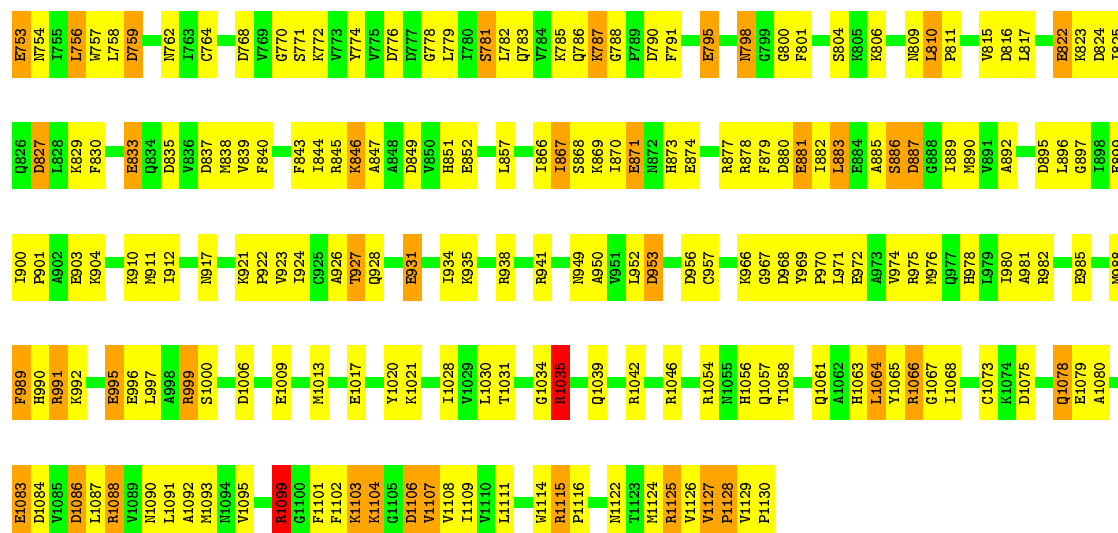
#### • Molecule 1: PYRUVATE KINASE



#### • Molecule 1: PYRUVATE KINASE

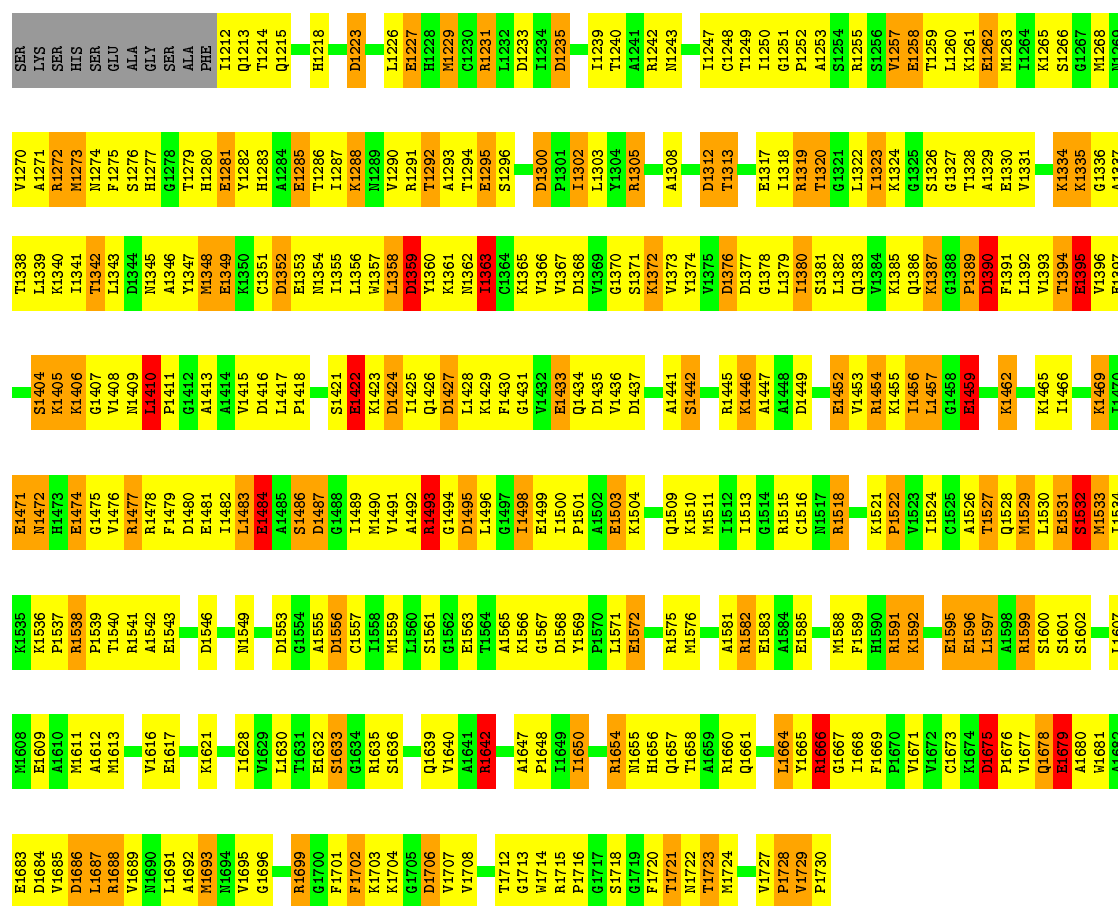






### • Molecule 1: PYRUVATE KINASE

Chain C: 32% 45% 17%



### • Molecule 1: PYRUVATE KINASE

Chain D: 45% 43% 9%

L2264	L2179	G2088	P2018	K1865	I2267	D2275	P2276	P2277	Q2278	E2279	A2280	W2281	E2282	D2283	V2285	D2286	L2287	R2288	L2291	A2292	R2293	R2294	T2295	G2296	R2299	F2302	K2303	K2304	G2305	D2306	V2307	V2308	L2311	T2312	R2315	P2316	G2317	G2319	T2321	N2322	T2323	R2324	R2325	V2326	P2330
Y2265	I2180	I2089	A2019	M1868	I2271	P2276	P2277	Q2278	E2279	A2280	W2281	E2282	D2283	V2285	D2286	L2287	R2288	L2291	A2292	R2293	R2294	T2295	G2296	R2299	F2302	K2303	K2304	G2305	D2306	V2307	V2308	L2311	T2312	R2315	P2316	G2317	G2319	T2321	N2322	T2323	R2324	R2325	V2326	P2330	
R2266	A2181	T2090	S2021	M1869	G2267	P2276	P2277	Q2278	E2279	A2280	W2281	E2282	D2283	V2285	D2286	L2287	R2288	L2291	A2292	R2293	R2294	T2295	G2296	R2299	F2302	K2303	K2304	G2305	D2306	V2307	V2308	L2311	T2312	R2315	P2316	G2317	G2319	T2321	N2322	T2323	R2324	R2325	V2326	P2330	
I2268	R2182	V2091	S2021	N1869	G2267	P2276	P2277	Q2278	E2279	A2280	W2281	E2282	D2283	V2285	D2286	L2287	R2288	L2291	A2292	R2293	R2294	T2295	G2296	R2299	F2302	K2303	K2304	G2305	D2306	V2307	V2308	L2311	T2312	R2315	P2316	G2317	G2319	T2321	N2322	T2323	R2324	R2325	V2326	P2330	
	E2185	R2093	K2023																																										
		D2094	D2024																																										
		D2095	I2025																																										
	E2099		D2027																																										
		E2103																																											
		Q2109	E2033																																										
		K2110	Q2034																																										
			D2035																																										
		I2113	D2036																																										
			D2037																																										
		C2116	M2038																																										
		R2117																																											
		A2119	A2041																																										
		G2120	F2043																																										
		K2121	I2044																																										
		F2122	R2045																																										
		A2126	K2046																																										
		T2127	A2047																																										
		Q2128	D2049																																										
		K2129																																											
		L2130	E2052																																										
		E2131	V2053																																										
		R2054	R1980																																										
		K2055	L1904																																										
		L2056	K1985																																										
		D2057	Q1986																																										
		P2139	K1987																																										
		T2140	E2059																																										
		R2141																																											
		A2142	K2062																																										
		E2143	N2063																																										
		G2144	I2064																																										
		S2145	K2065																																										
		D2146	I2066																																										
		A2155	L2067																																										
		D2156	K2069																																										
		K2166	N2072																																										
		G2167	R2077																																										
		D2168																																											
		Y2169	D2080																																										
		P2170	E2081																																										
		L2171	I2082																																										
		E2172	L2083																																										
		A2173	E2084																																										
		R2175	A2085																																										
		K2176	D2086																																										
			D2087																																										

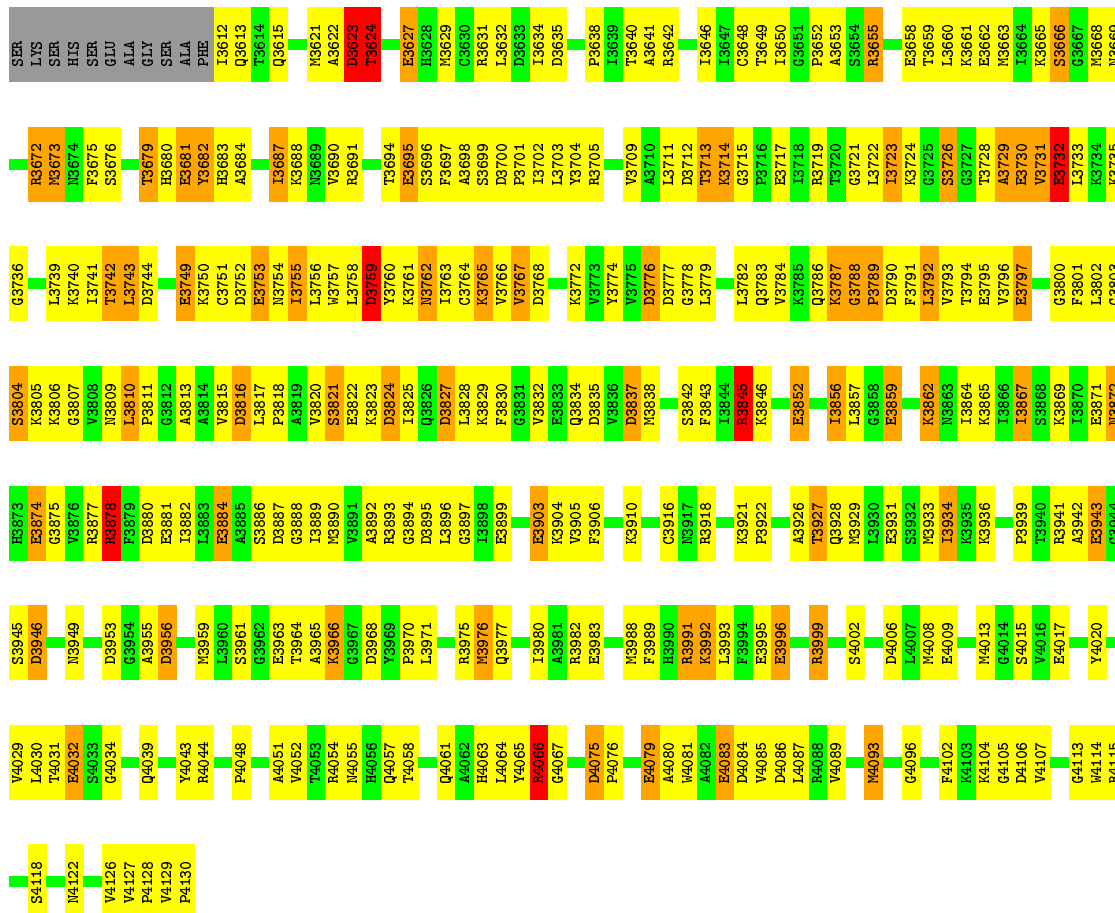
• Molecule 1: PYRUVATE KINASE

Chain E:  44% 39% 12% . .

Q3461	L3379	I3298	L3228	I3156	E3081	SER
A3462	E3299	E3299	K3229	W3157	H3083	LYS
H3463	L3380	L3380	F3230	L3158	H3083	SER
L3464	A3381	P3301		D3159	A3084	HIS
Y3465	E3382		E3233	T3160	E3085	SER
K3466	E3383	K3304	Q3234	K3161	T3086	GLU
G3467		V3305	D3235	N3162	I3087	GLY
L3468	F3389	F3306	D3236	I3163		ALA
F3469	H3390	L3307	D3237	C3164	R3091	SER
P3470	R3391			G3165		ALA
	K3392	K3311	S3242	V3166	E3095	PHE
D3475			F2443	V3167		I3012
P3476	E3395	R3315	L3244	D3168	S3099	Q3013
V3477	E3396	C3316	K3245		D3100	T3014
Q3478	L3397		K3246	S3171	P3101	Q3015
E3479	A3398	G3320		K3172	I3102	Q3016
R3480	R3399	K3321	D3249	V3173	L3103	L3017
K3481		P3322				E3018
A3482	S3402	V3323	E3252	D3176	P3106	A3019
E3483	D3406	I3324	V3253	D3177	V3107	A3020
D3484	L3407	T3327	K3254	G3178	A3021	H3022
	K3408	Q3328	R3255	L3179	V3109	Q3021
R3488	E3409	H3329	L3256	I3180	A3108	D3023
M3493	A3410	L3330	L3257	S3181		T3024
N3494	M3411	E3331	G3258	L3182	D3112	
V3495	A3412	S3332	E3259	Q3183	T3113	
G3496	M3413	R3333	K3262	Q3186	K3114	
K3497		L3334		K3187	G3115	
A3498	E3417	K3335	K3265	G3188	H3028	
R3499	K3421	R3337	I3266		M3029	
G3500		R3338	K3269	F3191	C3030	
F3501	A3425	P3339	T3270	L3192	R3031	
K3503	A3426	T3340	E3271	V3193		
K3504		R3341	K3272	T3194	A3041	
G3505	L3430	E3342	H3273	E3195	R3042	
R3506	T3431	E3343	E3274	V3196		
V3507	E3432		E3275	E3197	C3048	
V3508	S3433	D3346	V3276	N3198	T3049	
I3509	G3434	V3347	R3277		I3050	
	R3435		R3278	L3202	G3051	
		A3350	F3279			
W3514	V3440	V3351	D3280	K3205	S3054	
P3516	A3441	R3352	E3281	K3206	R3055	
	R3442	D3353	I3282	G3207	S3056	
		A3354	I3283	V3208	V3057	
N3522	R3446	A3355	E3284	N3209	E3058	
	A3447	D3356	A3285	L3210		
R3525	F3448	C3357	S3286	P3211	T3142	
V3527	I3449		D3287	D3144	L3143	
P3528		K3366	G3288	R3145	R3062	
V3529	V3452		L3289	A3146	S3066	
P3530	T3453		K3290	X3147	G3067	
			S3221		X3068	
			E3291			
			V3291			
			A3292			
			R3293			
			E3294			
			D3295			
				</		

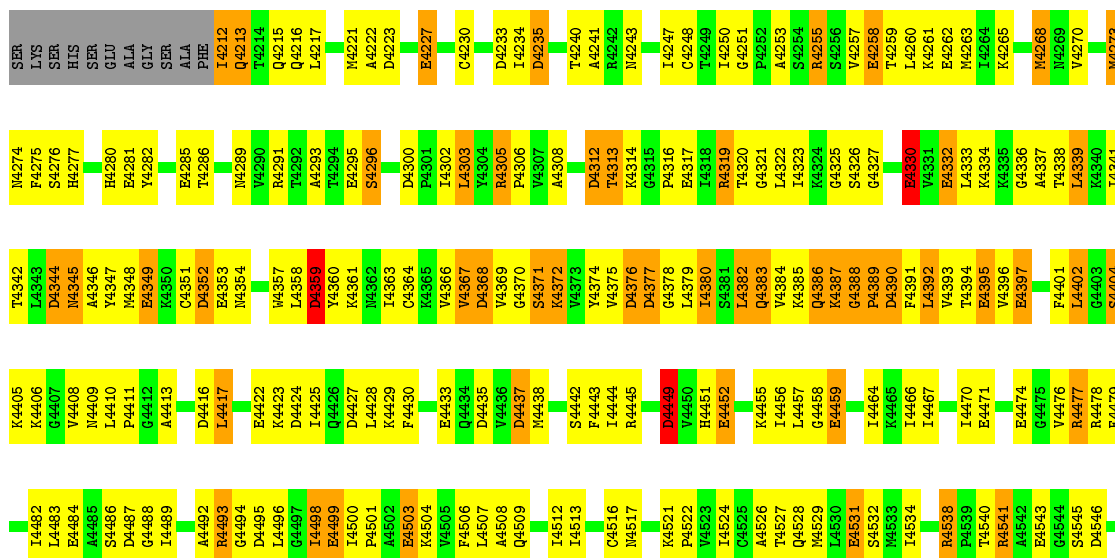
- Molecule 1: PYRUVATE KINASE

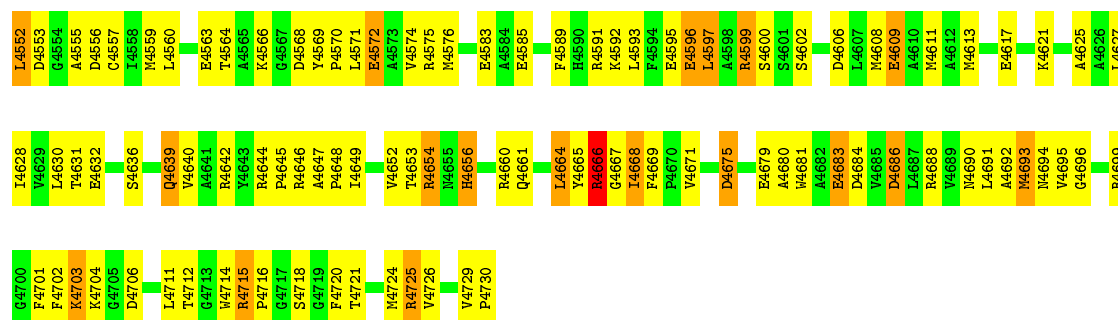
Chain F:



- Molecule 1: PYRUVATE KINASE

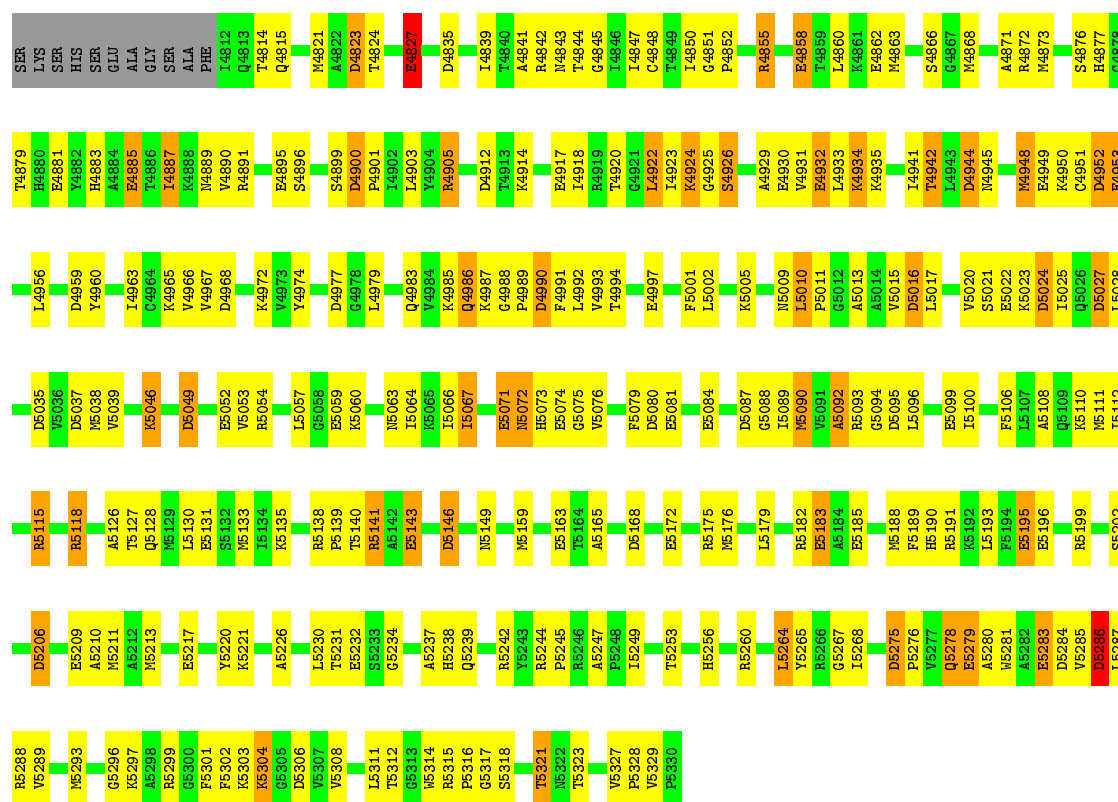
Chain G:





• Molecule 1: PYRUVATE KINASE

Chain H: 50% 39% 8%



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	95.30 Å   216.50 Å   258.60 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	30.00 – 2.35	Depositor
% Data completeness (in resolution range)	85.0 (30.00-2.35)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	TNT 5D	Depositor
R, $R_{free}$	0.190 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	33890	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: OXL, NA, MG, ATP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	1.06	31/4041 (0.8%)	1.39	57/5452 (1.0%)
1	B	1.02	25/4041 (0.6%)	1.39	59/5452 (1.1%)
1	C	0.98	26/4041 (0.6%)	1.39	66/5452 (1.2%)
1	D	1.01	29/4041 (0.7%)	1.39	56/5452 (1.0%)
1	E	1.01	29/4041 (0.7%)	1.43	63/5452 (1.2%)
1	F	0.97	24/4041 (0.6%)	1.40	62/5452 (1.1%)
1	G	0.99	30/4041 (0.7%)	1.39	60/5452 (1.1%)
1	H	1.01	29/4041 (0.7%)	1.37	62/5452 (1.1%)
All	All	1.00	223/32328 (0.7%)	1.39	485/43616 (1.1%)

All (223) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	162	ASN	N-CA	18.25	1.82	1.46
1	A	241	ALA	C-N	-8.32	1.15	1.34
1	D	1917	GLU	CD-OE2	8.30	1.34	1.25
1	B	681	GLU	CD-OE2	8.22	1.34	1.25
1	G	4595	GLU	CD-OE1	8.00	1.34	1.25
1	A	27	GLU	CD-OE2	7.88	1.34	1.25
1	B	627	GLU	CD-OE2	7.62	1.34	1.25
1	E	3222	GLU	CD-OE2	7.59	1.33	1.25
1	C	1595	GLU	CD-OE1	7.57	1.33	1.25
1	F	3797	GLU	CD-OE1	7.55	1.33	1.25
1	B	871	GLU	CD-OE2	7.52	1.33	1.25
1	H	5195	GLU	CD-OE1	7.45	1.33	1.25
1	C	1317	GLU	CD-OE2	7.29	1.33	1.25
1	G	4332	GLU	CD-OE2	7.29	1.33	1.25
1	D	2143	GLU	CD-OE2	7.28	1.33	1.25
1	B	795	GLU	CD-OE1	7.28	1.33	1.25
1	E	3195	GLU	CD-OE2	7.14	1.33	1.25
1	H	4997	GLU	CD-OE2	7.08	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	874	GLU	CD-OE1	7.05	1.33	1.25
1	H	4858	GLU	CD-OE2	7.00	1.33	1.25
1	A	222	GLU	CD-OE2	6.94	1.33	1.25
1	A	432	GLU	CD-OE2	6.90	1.33	1.25
1	D	2283	GLU	CD-OE1	6.88	1.33	1.25
1	C	1471	GLU	CD-OE2	6.84	1.33	1.25
1	G	4281	GLU	CD-OE2	6.79	1.33	1.25
1	G	4227	GLU	CD-OE2	6.76	1.33	1.25
1	H	5279	GLU	CD-OE2	6.75	1.33	1.25
1	G	4258	GLU	CD-OE1	6.74	1.33	1.25
1	E	3085	GLU	CD-OE1	6.72	1.33	1.25
1	E	3095	GLU	CD-OE1	6.67	1.32	1.25
1	A	385	GLU	CD-OE1	6.63	1.32	1.25
1	B	833	GLU	CD-OE2	6.61	1.32	1.25
1	D	2196	GLU	CD-OE1	6.59	1.32	1.25
1	E	3396	GLU	CD-OE1	6.57	1.32	1.25
1	A	483	GLU	CD-OE1	6.52	1.32	1.25
1	C	1531	GLU	CD-OE2	6.51	1.32	1.25
1	C	1459	GLU	CD-OE1	6.50	1.32	1.25
1	E	3081	GLU	CD-OE2	6.48	1.32	1.25
1	E	3299	GLU	CD-OE2	6.47	1.32	1.25
1	F	4079	GLU	CD-OE2	6.45	1.32	1.25
1	H	4881	GLU	CD-OE2	6.45	1.32	1.25
1	E	3149	GLU	CD-OE2	6.45	1.32	1.25
1	G	4285	GLU	CD-OE1	6.43	1.32	1.25
1	A	259	GLU	CD-OE1	6.42	1.32	1.25
1	B	852	GLU	CD-OE2	6.38	1.32	1.25
1	E	3027	GLU	CD-OE2	6.37	1.32	1.25
1	B	662	GLU	CD-OE2	6.35	1.32	1.25
1	B	1079	GLU	CD-OE2	6.35	1.32	1.25
1	B	685	GLU	CD-OE1	6.35	1.32	1.25
1	E	3259	GLU	CD-OE1	6.33	1.32	1.25
1	C	1499	GLU	CD-OE2	6.30	1.32	1.25
1	E	3331	GLU	CD-OE2	6.29	1.32	1.25
1	B	753	GLU	CD-OE2	6.26	1.32	1.25
1	C	1258	GLU	CD-OE2	6.24	1.32	1.25
1	F	3795	GLU	CD-OE1	6.23	1.32	1.25
1	G	4632	GLU	CD-OE2	6.22	1.32	1.25
1	E	3252	GLU	CD-OE1	6.20	1.32	1.25
1	A	303	GLU	CD-OE1	6.20	1.32	1.25
1	B	749	GLU	CD-OE2	6.20	1.32	1.25
1	F	3996	GLU	CD-OE1	6.19	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	85	GLU	CD-OE2	6.18	1.32	1.25
1	F	3874	GLU	CD-OE1	6.18	1.32	1.25
1	F	3695	GLU	CD-OE1	6.16	1.32	1.25
1	F	3730	GLU	CD-OE2	6.16	1.32	1.25
1	H	5059	GLU	CD-OE2	6.16	1.32	1.25
1	F	3627	GLU	CD-OE2	6.14	1.32	1.25
1	E	3432	GLU	CD-OE2	6.14	1.32	1.25
1	D	1858	GLU	CD-OE2	6.14	1.32	1.25
1	D	2033	GLU	CD-OE2	6.14	1.32	1.25
1	C	1353	GLU	CD-OE2	6.13	1.32	1.25
1	F	3871	GLU	CD-OE2	6.12	1.32	1.25
1	H	5283	GLU	CD-OE2	6.12	1.32	1.25
1	B	822	GLU	CD-OE2	6.12	1.32	1.25
1	D	2279	GLU	CD-OE2	6.12	1.32	1.25
1	B	658	GLU	CD-OE2	6.10	1.32	1.25
1	E	3062	GLU	CD-OE2	6.09	1.32	1.25
1	G	4422	GLU	CD-OE1	6.08	1.32	1.25
1	E	3281	GLU	CD-OE1	6.03	1.32	1.25
1	F	4017	GLU	CD-OE1	6.02	1.32	1.25
1	H	5143	GLU	CD-OE2	6.02	1.32	1.25
1	A	274	GLU	CD-OE1	6.02	1.32	1.25
1	E	3233	GLU	CD-OE2	5.99	1.32	1.25
1	G	4585	GLU	CD-OE1	5.99	1.32	1.25
1	H	4953	GLU	CD-OE2	5.98	1.32	1.25
1	D	2022	GLU	CD-OE2	5.98	1.32	1.25
1	G	4609	GLU	CD-OE2	5.98	1.32	1.25
1	F	3903	GLU	CD-OE1	5.97	1.32	1.25
1	C	1596	GLU	CD-OE1	5.96	1.32	1.25
1	B	695	GLU	CD-OE1	5.96	1.32	1.25
1	H	5099	GLU	CD-OE2	5.95	1.32	1.25
1	G	4679	GLU	CD-OE2	5.94	1.32	1.25
1	C	1572	GLU	CD-OE1	5.93	1.32	1.25
1	D	1827	GLU	CD-OE2	5.92	1.32	1.25
1	C	1281	GLU	CD-OE1	5.91	1.32	1.25
1	G	4349	GLU	CD-OE2	5.91	1.32	1.25
1	B	1083	GLU	CD-OE2	5.90	1.32	1.25
1	H	4949	GLU	CD-OE2	5.90	1.32	1.25
1	D	2103	GLU	CD-OE1	5.90	1.32	1.25
1	A	252	GLU	CD-OE2	5.89	1.32	1.25
1	C	1395	GLU	CD-OE1	5.88	1.32	1.25
1	G	4572	GLU	CD-OE1	5.87	1.32	1.25
1	E	3271	GLU	CD-OE2	5.86	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	331	GLU	CD-OE2	5.86	1.32	1.25
1	A	479	GLU	CD-OE2	5.85	1.32	1.25
1	G	4317	GLU	CD-OE2	5.85	1.32	1.25
1	B	899	GLU	CD-OE2	5.84	1.32	1.25
1	C	1632	GLU	CD-OE2	5.83	1.32	1.25
1	A	395	GLU	CD-OE1	5.83	1.32	1.25
1	B	985	GLU	CD-OE1	5.81	1.32	1.25
1	A	95	GLU	CD-OE1	5.81	1.32	1.25
1	C	1679	GLU	CD-OE2	5.80	1.32	1.25
1	E	3058	GLU	CD-OE1	5.80	1.32	1.25
1	D	2059	GLU	CD-OE1	5.77	1.31	1.25
1	D	2232	GLU	CD-OE1	5.76	1.31	1.25
1	G	4262	GLU	CD-OE2	5.76	1.31	1.25
1	A	58	GLU	CD-OE2	5.76	1.31	1.25
1	C	1330	GLU	CD-OE2	5.75	1.31	1.25
1	F	3995	GLU	CD-OE1	5.75	1.31	1.25
1	C	1503	GLU	CD-OE1	5.75	1.31	1.25
1	E	3372	GLU	CD-OE1	5.74	1.31	1.25
1	F	3749	GLU	CD-OE2	5.73	1.31	1.25
1	A	396	GLU	CD-OE1	5.72	1.31	1.25
1	E	3383	GLU	CD-OE2	5.71	1.31	1.25
1	F	3943	GLU	CD-OE2	5.71	1.31	1.25
1	B	995	GLU	CD-OE2	5.71	1.31	1.25
1	H	5022	GLU	CD-OE2	5.70	1.31	1.25
1	C	1452	GLU	CD-OE2	5.67	1.31	1.25
1	B	931	GLU	CD-OE2	5.67	1.31	1.25
1	D	1895	GLU	CD-OE1	5.67	1.31	1.25
1	B	717	GLU	CD-OE2	5.66	1.31	1.25
1	E	3479	GLU	CD-OE2	5.66	1.31	1.25
1	A	409	GLU	CD-OE2	5.65	1.31	1.25
1	E	3417	GLU	CD-OE1	5.65	1.31	1.25
1	H	4862	GLU	CD-OE2	5.64	1.31	1.25
1	D	2052	GLU	CD-OE1	5.64	1.31	1.25
1	G	4353	GLU	CD-OE2	5.62	1.31	1.25
1	G	4452	GLU	CD-OE2	5.60	1.31	1.25
1	H	5232	GLU	CD-OE1	5.60	1.31	1.25
1	D	1932	GLU	CD-OE1	5.60	1.31	1.25
1	C	1683	GLU	CD-OE1	5.60	1.31	1.25
1	D	1949	GLU	CD-OE2	5.60	1.31	1.25
1	E	3483	GLU	CD-OE2	5.58	1.31	1.25
1	B	730	GLU	CD-OE2	5.57	1.31	1.25
1	E	3132	GLU	CD-OE1	5.57	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	4683	GLU	CD-OE1	5.57	1.31	1.25
1	C	1285	GLU	CD-OE1	5.56	1.31	1.25
1	H	5131	GLU	CD-OE1	5.55	1.31	1.25
1	G	4433	GLU	CD-OE2	5.54	1.31	1.25
1	A	363	GLU	CD-OE1	5.54	1.31	1.25
1	A	343	GLU	CD-OE2	5.53	1.31	1.25
1	D	2131	GLU	CD-OE1	5.53	1.31	1.25
1	G	4484	GLU	CD-OE1	5.52	1.31	1.25
1	C	1484	GLU	CD-OE2	5.52	1.31	1.25
1	D	2084	GLU	CD-OE2	5.52	1.31	1.25
1	F	3658	GLU	CD-OE2	5.51	1.31	1.25
1	H	5196	GLU	CD-OE1	5.50	1.31	1.25
1	E	3284	GLU	CD-OE2	5.50	1.31	1.25
1	A	62	GLU	CD-OE1	5.49	1.31	1.25
1	H	4930	GLU	CD-OE2	5.49	1.31	1.25
1	G	4531	GLU	CD-OE2	5.46	1.31	1.25
1	F	3852	GLU	CD-OE2	5.46	1.31	1.25
1	A	132	GLU	CD-OE1	5.45	1.31	1.25
1	D	2172	GLU	CD-OE2	5.45	1.31	1.25
1	F	3963	GLU	CD-OE1	5.45	1.31	1.25
1	D	1997	GLU	CD-OE2	5.45	1.31	1.25
1	D	1930	GLU	CD-OE2	5.44	1.31	1.25
1	F	3859	GLU	CD-OE1	5.43	1.31	1.25
1	D	1995	GLU	CD-OE1	5.42	1.31	1.25
1	E	3117	GLU	CD-OE2	5.41	1.31	1.25
1	G	4459	GLU	CD-OE2	5.41	1.31	1.25
1	F	3732	GLU	CD-OE1	5.41	1.31	1.25
1	F	3753	GLU	CD-OE2	5.40	1.31	1.25
1	H	5172	GLU	CD-OE1	5.39	1.31	1.25
1	H	4895	GLU	CD-OE1	5.38	1.31	1.25
1	H	5074	GLU	CD-OE1	5.38	1.31	1.25
1	C	1262	GLU	CD-OE2	5.37	1.31	1.25
1	H	4885	GLU	CD-OE2	5.35	1.31	1.25
1	H	4827	GLU	CD-OE1	5.35	1.31	1.25
1	B	881	GLU	CD-OE2	5.35	1.31	1.25
1	F	3681	GLU	CD-OE2	5.34	1.31	1.25
1	G	4330	GLU	CD-OE2	5.34	1.31	1.25
1	A	281	GLU	CD-OE2	5.34	1.31	1.25
1	C	1349	GLU	CD-OE2	5.33	1.31	1.25
1	A	233	GLU	CD-OE1	5.33	1.31	1.25
1	G	4397	GLU	CD-OE2	5.32	1.31	1.25
1	H	5163	GLU	CD-OE1	5.32	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	4617	GLU	CD-OE2	5.32	1.31	1.25
1	A	372	GLU	CD-OE1	5.29	1.31	1.25
1	H	5217	GLU	CD-OE2	5.29	1.31	1.25
1	D	1862	GLU	CD-OE2	5.28	1.31	1.25
1	D	1881	GLU	CD-OE2	5.28	1.31	1.25
1	C	1422	GLU	CD-OE1	5.27	1.31	1.25
1	F	4083	GLU	CD-OE1	5.27	1.31	1.25
1	A	153	GLU	CD-OE2	5.27	1.31	1.25
1	H	5052	GLU	CD-OE2	5.26	1.31	1.25
1	G	4563	GLU	CD-OE1	5.25	1.31	1.25
1	H	5084	GLU	CD-OE2	5.25	1.31	1.25
1	D	1953	GLU	CD-OE2	5.24	1.31	1.25
1	B	1017	GLU	CD-OE1	5.24	1.31	1.25
1	A	197	GLU	CD-OE2	5.23	1.31	1.25
1	F	3884	GLU	CD-OE2	5.22	1.31	1.25
1	H	4917	GLU	CD-OE1	5.22	1.31	1.25
1	G	4295	GLU	CD-OE2	5.20	1.31	1.25
1	D	2209	GLU	CD-OE1	5.18	1.31	1.25
1	F	3822	GLU	CD-OE2	5.17	1.31	1.25
1	G	4499	GLU	CD-OE2	5.17	1.31	1.25
1	C	1617	GLU	CD-OE1	5.17	1.31	1.25
1	E	3274	GLU	CD-OE1	5.17	1.31	1.25
1	E	3409	GLU	CD-OE2	5.16	1.31	1.25
1	C	1474	GLU	CD-OE2	5.16	1.31	1.25
1	D	2217	GLU	CD-OE1	5.15	1.31	1.25
1	D	2185	GLU	CD-OE2	-5.12	1.20	1.25
1	A	299	GLU	CD-OE2	5.12	1.31	1.25
1	B	903	GLU	CD-OE1	5.12	1.31	1.25
1	G	4503	GLU	CD-OE1	5.11	1.31	1.25
1	G	4596	GLU	CD-OE1	5.09	1.31	1.25
1	A	81	GLU	CD-OE1	5.07	1.31	1.25
1	H	5071	GLU	CD-OE2	5.07	1.31	1.25
1	A	271	GLU	CD-OE2	5.05	1.31	1.25
1	D	2195	GLU	CD-OE1	5.04	1.31	1.25
1	E	3130	GLU	CD-OE2	5.02	1.31	1.25
1	H	5183	GLU	CD-OE2	5.02	1.31	1.25
1	C	1433	GLU	CD-OE2	5.01	1.31	1.25

All (485) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1919	ARG	NE-CZ-NH1	14.55	127.58	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1919	ARG	NE-CZ-NH2	-12.64	113.98	120.30
1	F	4066	ARG	NE-CZ-NH1	11.98	126.29	120.30
1	B	1127	VAL	C-N-CD	-11.61	95.06	120.60
1	A	164	CYS	O-C-N	11.47	141.05	122.70
1	E	3499	ARG	NE-CZ-NH1	10.93	125.76	120.30
1	A	162	ASN	N-CA-CB	-10.87	91.04	110.60
1	E	3224	ASP	CB-CG-OD1	-10.51	108.84	118.30
1	C	1666	ARG	NE-CZ-NH2	-10.24	115.18	120.30
1	H	4835	ASP	CB-CG-OD1	-10.22	109.10	118.30
1	E	3245	ARG	NE-CZ-NH1	9.83	125.21	120.30
1	E	3176	ASP	CB-CG-OD1	-9.67	109.59	118.30
1	E	3119	ARG	NE-CZ-NH1	9.67	125.14	120.30
1	F	3776	ASP	CB-CG-OD1	-9.20	110.02	118.30
1	F	3788	GLY	C-N-CD	-9.14	100.48	120.60
1	C	1666	ARG	NE-CZ-NH1	9.08	124.84	120.30
1	E	3176	ASP	CB-CG-OD2	9.07	126.47	118.30
1	H	5087	ASP	CB-CG-OD2	-9.03	110.17	118.30
1	F	3712	ASP	CB-CG-OD1	-9.02	110.19	118.30
1	C	1427	ASP	CB-CG-OD1	-8.94	110.26	118.30
1	G	4449	ASP	CB-CG-OD1	8.88	126.30	118.30
1	A	506	ASP	CB-CG-OD2	8.85	126.26	118.30
1	C	1368	ASP	CB-CA-C	-8.83	92.74	110.40
1	D	1831	ARG	NE-CZ-NH1	8.77	124.68	120.30
1	E	3356	ASP	CB-CG-OD1	-8.74	110.44	118.30
1	B	956	ASP	CB-CG-OD2	-8.70	110.47	118.30
1	B	837	ASP	CB-CG-OD1	-8.62	110.54	118.30
1	E	3168	ASP	CB-CG-OD2	-8.62	110.55	118.30
1	G	4541	ARG	NE-CZ-NH1	8.41	124.51	120.30
1	D	2087	ASP	CB-CG-OD2	-8.40	110.74	118.30
1	A	506	ASP	CB-CG-OD1	-8.38	110.76	118.30
1	C	1688	ARG	NE-CZ-NH1	8.36	124.48	120.30
1	H	5027	ASP	CB-CG-OD1	-8.27	110.86	118.30
1	B	953	ASP	CB-CG-OD1	-8.21	110.91	118.30
1	E	3224	ASP	CB-CG-OD2	8.13	125.61	118.30
1	D	2035	ASP	CB-CG-OD2	8.10	125.59	118.30
1	G	4556	ASP	CB-CG-OD2	-8.09	111.02	118.30
1	A	164	CYS	CA-C-N	-8.08	99.42	117.20
1	G	4449	ASP	CB-CG-OD2	-7.96	111.13	118.30
1	B	953	ASP	CB-CG-OD2	7.95	125.45	118.30
1	G	4305	ARG	NE-CZ-NH1	7.94	124.27	120.30
1	H	4968	ASP	CB-CG-OD2	-7.92	111.17	118.30
1	E	3177	ASP	CB-CG-OD1	-7.88	111.20	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	3254	ARG	NE-CZ-NH1	7.88	124.24	120.30
1	H	4952	ASP	CB-CG-OD2	-7.82	111.26	118.30
1	G	4699	ARG	NE-CZ-NH1	7.73	124.16	120.30
1	B	668	MET	CG-SD-CE	-7.72	87.85	100.20
1	D	2095	ASP	CB-CG-OD1	-7.70	111.37	118.30
1	E	3152	ASP	CB-CG-OD2	-7.64	111.42	118.30
1	A	35	ASP	CB-CG-OD1	-7.64	111.43	118.30
1	D	1952	ASP	CB-CG-OD1	7.62	125.16	118.30
1	E	3152	ASP	CB-CG-OD1	7.62	125.16	118.30
1	D	2095	ASP	CB-CG-OD2	7.62	125.16	118.30
1	H	4835	ASP	CB-CG-OD2	7.59	125.13	118.30
1	G	4368	ASP	CB-CG-OD1	7.57	125.11	118.30
1	C	1493	ARG	NE-CZ-NH2	-7.49	116.56	120.30
1	G	4684	ASP	CB-CG-OD1	-7.44	111.60	118.30
1	G	4493	ARG	NE-CZ-NH1	7.44	124.02	120.30
1	H	5299	ARG	NE-CZ-NH2	-7.43	116.58	120.30
1	E	3216	ASP	CB-CG-OD2	-7.43	111.61	118.30
1	F	3623	ASP	CB-CG-OD2	7.42	124.97	118.30
1	B	705	ARG	NE-CZ-NH2	7.41	124.01	120.30
1	E	3210	LEU	C-N-CD	-7.41	104.30	120.60
1	A	499	ARG	NE-CZ-NH2	7.41	124.00	120.30
1	H	4842	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	G	4669	PHE	CB-CG-CD1	-7.35	115.65	120.80
1	F	4106	ASP	CB-CG-OD2	7.35	124.92	118.30
1	E	3023	ASP	CB-CG-OD2	-7.33	111.70	118.30
1	B	816	ASP	CB-CG-OD1	-7.33	111.70	118.30
1	A	235	ASP	CB-CG-OD2	7.33	124.89	118.30
1	B	1099	ARG	NE-CZ-NH2	7.33	123.96	120.30
1	B	956	ASP	CB-CG-OD1	7.32	124.89	118.30
1	G	4223	ASP	CB-CG-OD1	7.31	124.88	118.30
1	B	880	ASP	CB-CG-OD1	-7.30	111.73	118.30
1	G	4684	ASP	CB-CG-OD2	7.29	124.86	118.30
1	D	2299	ARG	NE-CZ-NH2	7.29	123.94	120.30
1	E	3295	ASP	CB-CG-OD1	-7.29	111.74	118.30
1	E	3249	ASP	CB-CG-OD1	7.28	124.85	118.30
1	B	719	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	H	5168	ASP	CB-CG-OD1	-7.28	111.75	118.30
1	C	1699	ARG	NE-CZ-NH2	7.28	123.94	120.30
1	G	4352	ASP	CB-CG-OD2	-7.26	111.77	118.30
1	B	1106	ASP	CB-CG-OD2	7.26	124.83	118.30
1	B	837	ASP	CB-CG-OD2	7.23	124.80	118.30
1	B	776	ASP	CB-CG-OD1	-7.22	111.80	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	2045	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	G	4352	ASP	CB-CG-OD1	7.21	124.79	118.30
1	A	368	ASP	CB-CG-OD2	-7.21	111.81	118.30
1	G	4312	ASP	CB-CG-OD1	-7.21	111.81	118.30
1	H	4944	ASP	CB-CG-OD1	-7.19	111.83	118.30
1	D	2035	ASP	CB-CG-OD1	-7.18	111.83	118.30
1	B	849	ASP	CB-CG-OD1	7.18	124.76	118.30
1	A	382	ARG	NE-CZ-NH2	7.16	123.88	120.30
1	D	1959	ASP	CB-CG-OD2	-7.14	111.88	118.30
1	F	3827	ASP	CB-CG-OD1	-7.13	111.88	118.30
1	H	5037	ASP	CB-CG-OD1	-7.13	111.89	118.30
1	F	3880	ASP	CB-CG-OD1	-7.13	111.89	118.30
1	D	1842	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	E	3035	ASP	CB-CG-OD2	-7.12	111.89	118.30
1	G	4291	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	H	5175	ARG	NE-CZ-NH2	-7.11	116.75	120.30
1	E	3023	ASP	CB-CG-OD1	7.11	124.70	118.30
1	F	3768	ASP	CB-CG-OD2	-7.09	111.92	118.30
1	C	1454	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	A	144	ASP	CB-CG-OD1	-7.07	111.93	118.30
1	E	3168	ASP	CB-CG-OD1	7.07	124.67	118.30
1	D	1919	ARG	CD-NE-CZ	7.07	133.50	123.60
1	C	1437	ASP	CB-CG-OD1	-7.07	111.94	118.30
1	C	1675	ASP	CB-CG-OD2	-7.07	111.94	118.30
1	C	1352	ASP	CB-CG-OD2	-7.06	111.95	118.30
1	F	3895	ASP	CB-CG-OD2	7.06	124.65	118.30
1	H	5284	ASP	CB-CG-OD1	-7.04	111.97	118.30
1	H	5206	ASP	CB-CG-OD2	-7.03	111.97	118.30
1	A	293	ARG	NE-CZ-NH1	7.03	123.81	120.30
1	C	1352	ASP	CB-CG-OD1	7.02	124.62	118.30
1	F	3845	ARG	NE-CZ-NH1	7.01	123.81	120.30
1	H	5288	ARG	NE-CZ-NH2	-7.01	116.80	120.30
1	E	3249	ASP	CB-CG-OD2	-6.98	112.02	118.30
1	H	4952	ASP	CB-CG-OD1	6.98	124.58	118.30
1	E	3177	ASP	CB-CG-OD2	6.97	124.57	118.30
1	F	3672	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	D	2146	ASP	CB-CG-OD1	-6.96	112.04	118.30
1	F	3712	ASP	CB-CG-OD2	6.94	124.55	118.30
1	B	880	ASP	CB-CG-OD2	6.94	124.55	118.30
1	D	2016	ASP	CB-CG-OD1	-6.93	112.06	118.30
1	C	1376	ASP	CB-CG-OD1	-6.93	112.06	118.30
1	A	318	ARG	NE-CZ-NH2	6.92	123.76	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	4912	ASP	CB-CG-OD1	-6.91	112.08	118.30
1	B	1084	ASP	CB-CG-OD1	-6.90	112.09	118.30
1	H	5087	ASP	CB-CG-OD1	6.89	124.50	118.30
1	B	712	ASP	CB-CG-OD2	6.88	124.50	118.30
1	A	391	ARG	NE-CZ-NH2	6.88	123.74	120.30
1	D	2175	ARG	NE-CZ-NH1	6.87	123.74	120.30
1	H	4990	ASP	CB-CG-OD2	6.87	124.48	118.30
1	B	1075	ASP	CB-CG-OD2	-6.86	112.12	118.30
1	A	346	ASP	CB-CG-OD2	6.86	124.47	118.30
1	B	887	ASP	CB-CG-OD2	-6.85	112.14	118.30
1	H	4968	ASP	CB-CG-OD1	6.84	124.46	118.30
1	E	3315	ARG	NE-CZ-NH1	6.83	123.71	120.30
1	A	368	ASP	CB-CG-OD1	6.82	124.44	118.30
1	E	3499	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	D	2199	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	H	5027	ASP	CB-CG-OD2	6.80	124.42	118.30
1	D	2045	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	D	1952	ASP	CB-CG-OD2	-6.79	112.19	118.30
1	C	1675	ASP	CB-CG-OD1	6.77	124.39	118.30
1	E	3216	ASP	CB-CG-OD1	6.73	124.36	118.30
1	D	2266	ARG	NE-CZ-NH2	-6.73	116.94	120.30
1	G	4223	ASP	CB-CG-OD2	-6.72	112.25	118.30
1	D	2087	ASP	CB-CG-OD1	6.72	124.35	118.30
1	F	3624	THR	N-CA-CB	-6.72	97.54	110.30
1	G	4312	ASP	CB-CG-OD2	6.69	124.32	118.30
1	B	968	ASP	CB-CG-OD1	-6.68	112.29	118.30
1	B	835	ASP	CB-CG-OD1	-6.68	112.29	118.30
1	F	4106	ASP	CB-CG-OD1	-6.67	112.30	118.30
1	E	3287	ASP	CB-CG-OD2	-6.66	112.31	118.30
1	E	3295	ASP	CB-CG-OD2	6.66	124.29	118.30
1	B	700	ASP	CB-CG-OD1	-6.63	112.33	118.30
1	A	315	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	F	3837	ASP	CB-CG-OD1	-6.62	112.34	118.30
1	C	1686	ASP	CB-CG-OD1	-6.61	112.35	118.30
1	A	249	ASP	CB-CG-OD2	-6.60	112.36	118.30
1	C	1556	ASP	CB-CG-OD2	6.60	124.24	118.30
1	B	895	ASP	CB-CG-OD1	-6.59	112.37	118.30
1	H	4990	ASP	CB-CG-OD1	-6.58	112.37	118.30
1	F	4086	ASP	CB-CG-OD1	-6.58	112.38	118.30
1	D	2080	ASP	CB-CG-OD1	-6.57	112.39	118.30
1	C	1546	ASP	CB-CG-OD2	6.56	124.21	118.30
1	A	100	ASP	CB-CG-OD1	-6.55	112.40	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	4075	ASP	CB-CG-OD2	-6.55	112.40	118.30
1	C	1480	ASP	CB-CG-OD1	-6.55	112.41	118.30
1	E	3119	ARG	NE-CZ-NH2	-6.51	117.05	120.30
1	G	4424	ASP	CB-CG-OD2	6.50	124.15	118.30
1	F	3759	ASP	CB-CG-OD1	-6.50	112.45	118.30
1	E	3435	ARG	NE-CZ-NH2	-6.49	117.05	120.30
1	F	3956	ASP	CB-CG-OD1	-6.48	112.46	118.30
1	F	3631	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	E	3475	ASP	CB-CG-OD1	-6.47	112.48	118.30
1	F	3968	ASP	CB-CG-OD1	-6.47	112.48	118.30
1	A	486	ASP	CB-CG-OD1	-6.46	112.48	118.30
1	A	216	ASP	CB-CG-OD1	-6.45	112.50	118.30
1	C	1556	ASP	CB-CG-OD1	-6.45	112.50	118.30
1	B	635	ASP	CB-CG-OD1	-6.44	112.50	118.30
1	B	776	ASP	CB-CG-OD2	6.44	124.09	118.30
1	B	849	ASP	CB-CG-OD2	-6.44	112.51	118.30
1	B	752	ASP	CB-CG-OD1	6.43	124.09	118.30
1	G	4706	ASP	CB-CG-OD2	6.43	124.08	118.30
1	F	3991	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	H	5146	ASP	CB-CG-OD2	6.40	124.06	118.30
1	H	5275	ASP	CB-CG-OD2	-6.40	112.54	118.30
1	D	1959	ASP	CB-CG-OD1	6.40	124.06	118.30
1	B	712	ASP	CB-CG-OD1	-6.39	112.55	118.30
1	D	1912	ASP	CB-CG-OD2	6.38	124.05	118.30
1	D	2306	ASP	CB-CG-OD1	6.38	124.05	118.30
1	A	399	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	C	1235	ASP	CB-CG-OD1	-6.38	112.56	118.30
1	F	4084	ASP	CB-CG-OD1	-6.37	112.57	118.30
1	B	623	ASP	CB-CG-OD2	-6.36	112.58	118.30
1	C	1493	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	F	3824	ASP	CB-CG-OD2	6.36	124.02	118.30
1	D	1912	ASP	CB-CG-OD1	-6.35	112.58	118.30
1	F	3946	ASP	CB-CG-OD1	-6.34	112.59	118.30
1	B	1035	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	D	2156	ASP	CB-CG-OD2	-6.33	112.60	118.30
1	G	4606	ASP	CB-CG-OD1	6.31	123.98	118.30
1	H	5024	ASP	CB-CG-OD2	-6.31	112.62	118.30
1	G	4235	ASP	CB-CG-OD1	-6.30	112.62	118.30
1	H	5016	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	A	484	ASP	CB-CG-OD1	-6.29	112.64	118.30
1	E	3356	ASP	CB-CG-OD2	6.28	123.95	118.30
1	A	235	ASP	CB-CG-OD1	-6.27	112.66	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	4115	ARG	NE-CZ-NH1	6.27	123.43	120.30
1	F	3790	ASP	CB-CG-OD2	-6.25	112.68	118.30
1	F	4084	ASP	CB-CG-OD2	6.23	123.91	118.30
1	A	486	ASP	CB-CG-OD2	6.23	123.91	118.30
1	B	790	ASP	CB-CG-OD1	-6.23	112.69	118.30
1	F	3768	ASP	CB-CG-OD1	6.23	123.91	118.30
1	G	4376	ASP	CB-CG-OD1	-6.22	112.70	118.30
1	A	23	ASP	CB-CG-OD2	-6.21	112.71	118.30
1	C	1599	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	G	4675	ASP	CB-CG-OD1	-6.21	112.71	118.30
1	D	2080	ASP	CB-CG-OD2	6.21	123.89	118.30
1	D	2141	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	F	3635	ASP	CB-CG-OD2	6.20	123.88	118.30
1	A	152	ASP	CB-CG-OD1	6.20	123.88	118.30
1	E	3235	ASP	CB-CG-OD2	6.19	123.88	118.30
1	B	635	ASP	CB-CG-OD2	6.19	123.87	118.30
1	B	1006	ASP	CB-CG-OD2	-6.18	112.73	118.30
1	H	4959	ASP	CB-CG-OD2	-6.18	112.73	118.30
1	B	981	ALA	CB-CA-C	6.16	119.35	110.10
1	A	475	ASP	CB-CG-OD2	-6.14	112.77	118.30
1	B	631	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	F	3895	ASP	CB-CG-OD1	-6.13	112.78	118.30
1	H	5141	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	F	4086	ASP	CB-CG-OD2	6.11	123.80	118.30
1	C	1546	ASP	CB-CG-OD1	-6.11	112.80	118.30
1	C	1568	ASP	CB-CG-OD1	-6.10	112.81	118.30
1	C	1427	ASP	CB-CG-OD2	6.08	123.78	118.30
1	A	406	ASP	CB-CG-OD2	-6.08	112.83	118.30
1	B	1106	ASP	CB-CG-OD1	-6.07	112.83	118.30
1	B	999	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	H	5138	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	H	5284	ASP	CB-CG-OD2	6.06	123.76	118.30
1	H	5168	ASP	CB-CG-OD2	6.05	123.75	118.30
1	C	1553	ASP	CB-CG-OD1	-6.04	112.86	118.30
1	G	4669	PHE	CB-CG-CD2	6.04	125.03	120.80
1	E	3399	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	H	4872	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	H	5090	MET	CG-SD-CE	-6.02	90.57	100.20
1	D	2138	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	E	3147	TYR	CA-CB-CG	-6.01	101.98	113.40
1	C	1729	VAL	C-N-CD	-6.01	107.38	120.60
1	B	968	ASP	CB-CG-OD2	6.01	123.71	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	4006	ASP	CB-CG-OD2	-6.00	112.90	118.30
1	F	3946	ASP	CB-CG-OD2	6.00	123.70	118.30
1	A	315	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	H	5288	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	D	1823	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	H	5141	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	D	1835	ASP	CB-CG-OD1	-5.98	112.92	118.30
1	H	5049	ASP	CB-CG-OD2	-5.98	112.92	118.30
1	F	3878	ARG	NE-CZ-NH1	5.97	123.28	120.30
1	H	5206	ASP	CB-CG-OD1	5.96	123.66	118.30
1	G	4377	ASP	CB-CG-OD2	5.95	123.66	118.30
1	C	1390	ASP	CB-CG-OD2	-5.95	112.95	118.30
1	C	1359	ASP	CB-CG-OD1	5.94	123.65	118.30
1	D	2146	ASP	CB-CG-OD2	5.94	123.64	118.30
1	A	295	ASP	CB-CG-OD2	5.93	123.64	118.30
1	G	4416	ASP	CB-CG-OD2	-5.93	112.96	118.30
1	C	1231	ARG	NE-CZ-NH2	-5.93	117.34	120.30
1	E	3278	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	B	827	ASP	CB-CG-OD1	-5.92	112.98	118.30
1	C	1495	ASP	CB-CG-OD1	-5.91	112.98	118.30
1	G	4725	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	A	466	ARG	NE-CZ-NH2	5.89	123.25	120.30
1	D	1990	ASP	CB-CG-OD1	5.89	123.60	118.30
1	B	759	ASP	CB-CA-C	-5.89	98.63	110.40
1	E	3035	ASP	CB-CG-OD1	5.88	123.59	118.30
1	G	4305	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	G	4568	ASP	CB-CG-OD2	5.88	123.59	118.30
1	A	254	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	G	4706	ASP	CB-CG-OD1	-5.87	113.02	118.30
1	B	991	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	A	152	ASP	CB-CG-OD2	-5.87	113.02	118.30
1	G	4686	ASP	CB-CG-OD1	-5.87	113.02	118.30
1	H	5037	ASP	CB-CG-OD2	5.86	123.57	118.30
1	E	3475	ASP	CB-CG-OD2	5.85	123.56	118.30
1	D	2016	ASP	CB-CG-OD2	5.84	123.56	118.30
1	H	5035	ASP	CB-CG-OD1	-5.84	113.04	118.30
1	F	4020	TYR	CB-CG-CD2	-5.83	117.50	121.00
1	D	2306	ASP	CB-CG-OD2	-5.82	113.06	118.30
1	F	3635	ASP	CB-CG-OD1	-5.82	113.06	118.30
1	C	1435	ASP	CB-CG-OD2	-5.81	113.07	118.30
1	F	3790	ASP	CB-CG-OD1	5.81	123.53	118.30
1	C	1480	ASP	CB-CG-OD2	5.80	123.52	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	346	ASP	CB-CG-OD1	-5.80	113.08	118.30
1	G	4388	GLY	C-N-CD	-5.80	107.84	120.60
1	G	4541	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	C	1686	ASP	CB-CG-OD2	5.79	123.52	118.30
1	F	3776	ASP	CB-CG-OD2	5.79	123.52	118.30
1	F	3816	ASP	CB-CG-OD1	-5.78	113.09	118.30
1	H	5035	ASP	CB-CG-OD2	5.78	123.50	118.30
1	H	5054	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	D	2275	ASP	CB-CG-OD1	-5.78	113.10	118.30
1	F	3744	ASP	CB-CG-OD1	-5.78	113.10	118.30
1	H	4977	ASP	CB-CG-OD1	-5.78	113.10	118.30
1	C	1272	ARG	NE-CZ-NH1	5.77	123.18	120.30
1	C	1642	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	H	4891	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	G	4606	ASP	CB-CG-OD2	-5.73	113.14	118.30
1	E	3406	ASP	CB-CG-OD1	-5.73	113.15	118.30
1	E	3164	CYS	O-C-N	5.71	131.84	122.70
1	C	1312	ASP	CB-CG-OD2	5.71	123.44	118.30
1	F	3887	ASP	CB-CG-OD1	5.70	123.43	118.30
1	B	1086	ASP	CB-CG-OD1	5.70	123.43	118.30
1	B	1020	TYR	CB-CG-CD2	-5.70	117.58	121.00
1	C	1435	ASP	CB-CG-OD1	5.70	123.42	118.30
1	G	4344	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	D	2315	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	F	3953	ASP	CB-CG-OD2	5.69	123.42	118.30
1	E	3100	ASP	CB-CG-OD2	5.69	123.42	118.30
1	E	3280	ASP	CB-CG-OD2	5.69	123.42	118.30
1	F	3953	ASP	CB-CG-OD1	-5.68	113.19	118.30
1	E	3066	SER	CB-CA-C	5.68	120.89	110.10
1	B	623	ASP	CB-CG-OD1	5.68	123.41	118.30
1	F	3682	TYR	CB-CG-CD1	-5.68	117.59	121.00
1	G	4553	ASP	CB-CG-OD1	-5.67	113.19	118.30
1	H	4959	ASP	CB-CG-OD1	5.67	123.41	118.30
1	A	295	ASP	CB-CG-OD1	-5.67	113.19	118.30
1	F	4006	ASP	CB-CG-OD1	5.67	123.40	118.30
1	C	1495	ASP	CB-CG-OD2	5.66	123.39	118.30
1	G	4654	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	C	1424	ASP	CB-CG-OD1	-5.66	113.21	118.30
1	C	1454	ARG	NE-CZ-NH1	5.65	123.13	120.30
1	E	3484	ASP	CB-CG-OD1	-5.65	113.21	118.30
1	E	3112	ASP	CB-CG-OD2	5.64	123.38	118.30
1	E	3484	ASP	CB-CG-OD2	5.64	123.38	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	3837	ASP	CB-CG-OD2	5.64	123.38	118.30
1	G	4538	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	B	1006	ASP	CB-CG-OD1	5.63	123.36	118.30
1	A	105	ARG	NE-CZ-NH2	5.63	123.11	120.30
1	G	4568	ASP	CB-CG-OD1	-5.63	113.23	118.30
1	B	1086	ASP	CB-CG-OD2	-5.62	113.24	118.30
1	D	2024	ASP	CB-CG-OD1	-5.62	113.24	118.30
1	E	3042	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	G	4686	ASP	CB-CG-OD2	5.62	123.36	118.30
1	H	5115	ARG	NE-CZ-NH2	-5.61	117.49	120.30
1	G	4675	ASP	CB-CG-OD2	5.61	123.35	118.30
1	C	1568	ASP	CB-CG-OD2	5.61	123.34	118.30
1	C	1591	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	H	5220	TYR	CB-CG-CD1	5.60	124.36	121.00
1	C	1223	ASP	CB-CG-OD2	-5.59	113.27	118.30
1	H	5275	ASP	CB-CG-OD1	5.59	123.33	118.30
1	C	1300	ASP	CB-CG-OD1	-5.59	113.27	118.30
1	D	1833	ASP	CB-CG-OD1	-5.58	113.28	118.30
1	D	1977	ASP	CB-CG-OD2	5.58	123.32	118.30
1	D	2175	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	G	4416	ASP	CB-CG-OD1	5.56	123.30	118.30
1	E	3346	ASP	CB-CG-OD1	-5.55	113.30	118.30
1	E	3382	ARG	N-CA-CB	5.55	120.59	110.60
1	H	5306	ASP	CB-CG-OD2	5.55	123.30	118.30
1	C	1312	ASP	CB-CG-OD1	-5.55	113.31	118.30
1	C	1449	ASP	CB-CG-OD1	5.54	123.29	118.30
1	E	3506	ASP	CB-CG-OD1	-5.54	113.31	118.30
1	A	406	ASP	CB-CG-OD1	5.54	123.29	118.30
1	D	2286	ASP	CB-CG-OD1	-5.54	113.32	118.30
1	G	4390	ASP	CB-CG-OD1	5.54	123.28	118.30
1	C	1231	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	F	3824	ASP	CB-CG-OD1	-5.53	113.32	118.30
1	B	824	ASP	CB-CG-OD1	-5.52	113.33	118.30
1	E	3112	ASP	CB-CG-OD1	-5.52	113.33	118.30
1	H	4823	ASP	CB-CG-OD1	-5.52	113.33	118.30
1	H	5323	THR	CA-CB-CG2	-5.52	104.68	112.40
1	B	700	ASP	CB-CG-OD2	5.51	123.26	118.30
1	A	508	VAL	N-CA-CB	-5.51	99.37	111.50
1	A	35	ASP	CB-CG-OD2	5.51	123.26	118.30
1	A	112	ASP	CB-CG-OD2	5.51	123.26	118.30
1	E	3245	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	G	4477	ARG	NE-CZ-NH1	5.48	123.04	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	673	MET	CG-SD-CE	5.47	108.96	100.20
1	G	4339	LEU	N-CA-CB	5.47	121.34	110.40
1	A	177	ASP	CB-CG-OD2	5.46	123.22	118.30
1	B	1075	ASP	CB-CG-OD1	5.46	123.22	118.30
1	A	484	ASP	CB-CG-OD2	5.45	123.21	118.30
1	D	1833	ASP	CB-CG-OD2	5.45	123.20	118.30
1	A	23	ASP	CB-CG-OD1	5.43	123.19	118.30
1	D	1904	TYR	CB-CG-CD2	-5.43	117.74	121.00
1	E	3072	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	F	3623	ASP	CB-CG-OD1	-5.42	113.42	118.30
1	D	2037	ASP	CB-CG-OD1	-5.41	113.43	118.30
1	F	3880	ASP	CB-CG-OD2	5.41	123.17	118.30
1	E	3159	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	H	4900	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	D	2168	ASP	CB-CG-OD1	5.40	123.16	118.30
1	G	4435	ASP	CB-CG-OD1	-5.39	113.45	118.30
1	H	4977	ASP	CB-CG-OD2	5.39	123.15	118.30
1	H	4823	ASP	CB-CG-OD2	5.39	123.15	118.30
1	C	1235	ASP	CB-CG-OD2	5.38	123.14	118.30
1	C	1242	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	D	1990	ASP	CB-CG-OD2	-5.38	113.46	118.30
1	A	112	ASP	CB-CG-OD1	-5.36	113.47	118.30
1	C	1223	ASP	CB-CG-OD1	5.36	123.13	118.30
1	C	1553	ASP	CB-CG-OD2	5.36	123.12	118.30
1	B	901	PRO	N-CA-CB	5.35	109.72	103.30
1	C	1449	ASP	CB-CG-OD2	-5.35	113.49	118.30
1	C	1437	ASP	CB-CG-OD2	5.34	123.11	118.30
1	C	1359	ASP	CB-CG-OD2	-5.34	113.50	118.30
1	E	3031	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	A	216	ASP	CB-CG-OD2	5.33	123.09	118.30
1	C	1377	ASP	CB-CG-OD1	-5.33	113.51	118.30
1	C	1688	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	H	5220	TYR	CB-CG-CD2	-5.32	117.81	121.00
1	G	4666	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	A	224	ASP	CB-CG-OD1	-5.31	113.52	118.30
1	A	254	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	F	3956	ASP	CB-CG-OD2	5.30	123.07	118.30
1	G	4642	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	D	2199	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	F	4020	TYR	CB-CG-CD1	5.29	124.17	121.00
1	H	5175	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	B	752	ASP	CB-CG-OD2	-5.29	113.54	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	4359	ASP	CB-CG-OD1	-5.28	113.55	118.30
1	C	1376	ASP	CB-CG-OD2	5.28	123.05	118.30
1	F	3877	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	B	744	ASP	CB-CG-OD1	-5.25	113.57	118.30
1	A	224	ASP	CB-CG-OD2	5.24	123.01	118.30
1	B	824	ASP	CB-CG-OD2	5.23	123.00	118.30
1	D	2266	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	H	5095	ASP	CB-CG-OD1	-5.22	113.61	118.30
1	H	4912	ASP	CB-CG-OD2	5.21	122.99	118.30
1	H	5095	ASP	CB-CG-OD2	5.21	122.99	118.30
1	F	3759	ASP	N-CA-CB	-5.21	101.22	110.60
1	F	3816	ASP	CB-CG-OD2	5.21	122.99	118.30
1	F	3835	ASP	CB-CG-OD2	5.21	122.99	118.30
1	H	5286	ASP	CB-CG-OD2	5.20	122.98	118.30
1	C	1424	ASP	CB-CG-OD2	5.20	122.98	118.30
1	C	1706	ASP	CB-CG-OD1	-5.20	113.62	118.30
1	H	5080	ASP	CB-CG-OD2	5.20	122.98	118.30
1	G	4437	ASP	CB-CG-OD2	5.19	122.97	118.30
1	E	3353	ASP	CB-CG-OD1	-5.18	113.64	118.30
1	G	4424	ASP	CB-CG-OD1	-5.17	113.64	118.30
1	A	176	ASP	CB-CG-OD1	-5.17	113.65	118.30
1	B	1115	ARG	CB-CA-C	5.17	120.73	110.40
1	H	4900	ASP	CB-CG-OD1	5.16	122.94	118.30
1	B	1088	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	E	3072	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	B	790	ASP	CB-CG-OD2	5.14	122.92	118.30
1	G	4688	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	A	176	ASP	CB-CG-OD2	5.13	122.92	118.30
1	C	1300	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	177	ASP	CB-CG-OD1	-5.13	113.68	118.30
1	C	1642	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	E	3338	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	F	3968	ASP	CB-CG-OD2	5.12	122.91	118.30
1	F	3682	TYR	CB-CG-CD2	5.12	124.07	121.00
1	E	3525	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	G	4487	ASP	CB-CG-OD1	5.11	122.90	118.30
1	A	144	ASP	CB-CG-OD2	5.11	122.90	118.30
1	E	3287	ASP	CB-CG-OD1	5.10	122.89	118.30
1	G	4359	ASP	CB-CA-C	-5.10	100.19	110.40
1	G	4553	ASP	CB-CG-OD2	5.09	122.88	118.30
1	H	4905	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	C	1487	ASP	CB-CG-OD2	-5.08	113.73	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	3227	ASP	CB-CG-OD2	5.07	122.86	118.30
1	C	1721	THR	CA-CB-CG2	-5.07	105.30	112.40
1	D	2244	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	G	4583	GLU	CG-CD-OE2	-5.07	108.16	118.30
1	G	4668	ILE	CA-CB-CG2	-5.07	100.77	110.90
1	E	3144	ASP	CB-CG-OD2	5.06	122.85	118.30
1	C	1233	ASP	CB-CG-OD1	-5.05	113.75	118.30
1	C	1654	ARG	NE-CZ-NH1	5.05	122.82	120.30
1	A	108	ALA	CB-CA-C	5.04	117.66	110.10
1	D	2275	ASP	CB-CG-OD2	5.04	122.84	118.30
1	A	227	ASP	CB-CG-OD2	5.04	122.83	118.30
1	F	3845	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	F	3777	ASP	CB-CG-OD1	-5.02	113.78	118.30
1	D	2206	ASP	CB-CG-OD2	5.01	122.81	118.30
1	A	100	ASP	CB-CG-OD2	5.01	122.81	118.30
1	A	287	ASP	CB-CG-OD2	-5.01	113.79	118.30
1	F	3759	ASP	CB-CA-C	-5.01	100.38	110.40
1	G	4339	LEU	CA-CB-CG	-5.01	103.78	115.30
1	G	4688	ARG	NE-CZ-NH1	5.01	122.80	120.30
1	D	2325	ARG	CB-CA-C	-5.00	100.39	110.40
1	E	3373	ALA	CB-CA-C	5.00	117.61	110.10
1	D	1831	ARG	NE-CZ-NH2	-5.00	117.80	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3978	0	4054	349	2
1	B	3978	0	4056	228	0
1	C	3978	0	4056	364	5
1	D	3978	0	4055	269	5
1	E	3978	0	4056	251	12
1	F	3978	0	4056	264	2
1	G	3978	0	4056	293	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	3978	0	4056	208	18
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	6	0	0	2	0
3	B	6	0	0	0	0
3	C	6	0	0	1	0
3	D	6	0	0	1	0
3	E	6	0	0	1	0
3	F	6	0	0	2	0
3	G	6	0	0	2	0
3	H	6	0	0	1	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
4	F	2	0	0	0	0
4	G	2	0	0	0	0
4	H	1	0	0	0	0
5	A	31	0	12	4	0
5	C	31	0	12	4	0
5	D	31	0	12	1	0
5	E	31	0	12	2	0
5	F	31	0	12	0	0
5	G	31	0	12	0	0
6	A	176	0	0	10	0
6	B	260	0	0	13	0
6	C	166	0	0	12	0
6	D	250	0	0	18	0
6	E	267	0	0	17	0
6	F	185	0	0	11	0
6	G	210	0	0	6	0
6	H	296	0	0	15	2
All	All	33890	0	32517	2117	24

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 33.



All (2117) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:ASN:N	1:A:162:ASN:CA	1.82	1.40
1:C:1678:GLN:HB2	1:C:1684:ASP:HB2	1.31	1.13
1:A:122:LEU:HD23	1:A:204:SER:HB3	1.28	1.12
1:E:3142:THR:HG22	1:E:3144:ASP:H	1.06	1.07
1:E:3493:MET:HE2	1:E:3530:PRO:HD2	1.37	1.06
1:A:326:ALA:HB1	1:A:359:MET:HE2	1.36	1.05
1:G:4665:TYR:HB2	1:G:4668:ILE:HD12	1.39	1.04
1:C:1248:CYS:HB2	1:C:1268:MET:HE3	1.38	1.04
1:B:650:ILE:HD11	1:B:668:MET:HE1	1.35	1.04
1:G:4250:ILE:HD11	1:G:4268:MET:HE1	1.41	1.02
1:H:5130:LEU:HD13	1:H:5133:MET:HE1	1.38	1.02
1:F:3624:THR:HG22	1:F:3627:GLU:H	1.18	1.01
1:A:514:TRP:H	1:A:522:ASN:HD21	1.10	1.00
1:D:1850:ILE:HD11	1:D:1868:MET:HE1	1.41	1.00
1:G:4367:VAL:HG22	1:G:4371:SER:HB3	1.43	1.00
1:H:4942:THR:HG23	1:H:4944:ASP:H	1.25	0.99
1:B:928:GLN:NE2	1:D:2141:ARG:H	1.60	0.99
1:A:141:ILE:HG21	1:A:158:LEU:HD22	1.44	0.98
1:A:113:THR:HG22	1:A:242:SER:HB2	1.40	0.98
1:A:126:SER:HB3	1:A:129:ALA:HB2	1.44	0.97
1:A:160:TYR:HD2	1:A:163:ILE:HB	1.28	0.97
1:A:51:GLY:O	1:A:55:ARG:HG3	1.65	0.97
1:D:2044:ILE:HG22	1:D:2082:ILE:HD12	1.47	0.96
1:F:3776:ASP:HB3	1:F:3779:LEU:HB3	1.47	0.95
1:H:5133:MET:HE2	1:H:5139:PRO:HG3	1.48	0.94
1:D:2176:MET:HA	1:D:2176:MET:HE3	1.47	0.93
1:F:3941:ARG:H	1:H:5128:GLN:HE21	1.15	0.93
1:E:3186:GLN:HB3	1:E:3193:VAL:HB	1.49	0.93
1:H:4848:CYS:HB2	1:H:4868:MET:HE3	1.50	0.92
1:C:1693:MET:HE2	1:C:1729:VAL:HG22	1.48	0.92
1:G:4322:LEU:HD23	1:G:4404:SER:HB2	1.51	0.92
1:C:1669:PHE:HB3	1:C:1699:ARG:HH12	1.32	0.92
1:G:4593:LEU:HD21	1:G:4644:ARG:HG3	1.52	0.91
1:A:431:THR:HG21	1:A:434:GLY:HA2	1.51	0.91
1:G:4250:ILE:HD11	1:G:4268:MET:CE	2.00	0.91
1:D:1824:THR:HG22	1:D:1827:GLU:HB2	1.50	0.90
1:E:3050:ILE:HD11	1:E:3068:MET:HE3	1.53	0.89
1:G:4680:ALA:HB3	1:G:4683:GLU:HG3	1.53	0.89
1:E:3341:ARG:H	1:G:4528:GLN:HE21	1.19	0.89
1:H:5020:VAL:HG13	1:H:5024:ASP:HB2	1.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1986:GLN:HB3	1:D:1993:VAL:HB	1.53	0.89
1:E:3048:CYS:HB2	1:E:3068:MET:HE3	1.53	0.89
1:F:3928:GLN:NE2	1:H:5141:ARG:H	1.71	0.89
1:B:1065:TYR:HB2	1:B:1068:ILE:HD12	1.53	0.89
1:C:1347:TYR:CD2	1:C:1355:ILE:HG21	2.07	0.88
1:C:1322:LEU:HD12	1:C:1349:GLU:HG2	1.53	0.88
1:C:1248:CYS:HB2	1:C:1268:MET:CE	2.03	0.88
1:G:4389:PRO:HD2	1:G:4391:PHE:CE2	2.08	0.88
1:H:4850:ILE:HD11	1:H:4868:MET:HE1	1.53	0.88
1:G:4371:SER:H	1:G:4384:VAL:HB	1.38	0.88
1:C:1382:LEU:HD21	1:C:1396:VAL:HG22	1.55	0.88
1:D:2090:MET:HE2	1:D:2092:ALA:HB2	1.56	0.88
1:B:815:VAL:HB	1:B:817:LEU:HD12	1.55	0.87
1:A:328:GLN:NE2	1:C:1541:ARG:H	1.72	0.87
1:D:1850:ILE:HB	1:D:1873:MET:HE3	1.57	0.87
1:C:1250:ILE:HB	1:C:1273:MET:HE3	1.57	0.87
1:H:5020:VAL:HG11	1:H:5025:ILE:HG12	1.56	0.87
1:C:1693:MET:CE	1:C:1729:VAL:HG22	2.05	0.87
1:F:3733:LEU:HD11	1:F:3802:LEU:HD22	1.57	0.87
1:H:5133:MET:HE2	1:H:5139:PRO:CG	2.05	0.87
1:F:3726:SER:HB3	1:F:3729:ALA:HB2	1.57	0.86
1:G:4367:VAL:HG22	1:G:4371:SER:CB	2.06	0.86
1:G:4479:PHE:CZ	1:G:4483:LEU:HD22	2.09	0.86
1:D:1850:ILE:HD11	1:D:1868:MET:CE	2.05	0.86
1:B:720:THR:HG22	1:B:758:LEU:CD2	2.04	0.86
1:E:3142:THR:HG22	1:E:3144:ASP:N	1.89	0.86
1:F:3928:GLN:HE21	1:H:5141:ARG:H	1.24	0.86
1:A:141:ILE:CG2	1:A:158:LEU:HD22	2.07	0.85
1:C:1591:ARG:HH12	1:C:1592:LYS:HE3	1.42	0.85
1:A:431:THR:CG2	1:A:434:GLY:HA2	2.06	0.85
1:E:3160:TYR:HD2	1:E:3163:ILE:HB	1.41	0.85
1:F:3949:ASN:HD21	1:H:5110:LYS:HZ1	1.24	0.85
1:C:1442:SER:HA	1:C:1469:LYS:HD3	1.59	0.84
1:E:3106:PRO:HG2	1:E:3470:PRO:HB2	1.60	0.84
1:E:3431:THR:HG21	1:E:3434:GLY:HA2	1.60	0.84
1:C:1678:GLN:HB2	1:C:1684:ASP:CB	2.08	0.84
1:H:4850:ILE:HD11	1:H:4868:MET:CE	2.08	0.83
1:G:4248:CYS:HB2	1:G:4268:MET:HE2	1.57	0.83
1:H:4926:SER:HB3	1:H:4929:ALA:H	1.42	0.83
1:H:5311:LEU:HB3	1:H:5321:THR:CG2	2.08	0.83
1:C:1343:LEU:HD21	1:C:1361:LYS:HA	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3050:ILE:HD11	1:E:3068:MET:CE	2.09	0.83
1:E:3376:MET:HA	1:E:3376:MET:HE3	1.61	0.83
1:E:3245:ARG:HB3	1:E:3274:GLU:HG2	1.58	0.83
1:A:118:ILE:CG2	1:A:208:VAL:HB	2.09	0.83
1:D:1824:THR:HG23	1:D:1827:GLU:H	1.44	0.83
1:E:3160:TYR:O	1:E:3163:ILE:HG22	1.78	0.83
1:B:1109:ILE:CD1	1:B:1126:VAL:HG22	2.09	0.82
1:B:928:GLN:HE21	1:D:2141:ARG:H	1.26	0.82
1:C:1534:ILE:HG23	1:C:1567:GLY:HA2	1.59	0.82
1:A:326:ALA:CB	1:A:359:MET:HE2	2.08	0.82
1:G:4248:CYS:HB2	1:G:4268:MET:CE	2.10	0.82
1:C:1343:LEU:CD2	1:C:1361:LYS:HA	2.10	0.82
1:A:301:PRO:HG2	1:A:304:LYS:HD2	1.61	0.81
1:D:2201:SER:HA	1:D:2203:HIS:CE1	2.14	0.81
1:B:648:CYS:HB2	1:B:668:MET:CE	2.10	0.81
1:D:2265:TYR:HB2	1:D:2268:ILE:HD12	1.61	0.81
1:C:1270:VAL:HG22	1:C:1308:ALA:HB3	1.60	0.81
1:C:1477:ARG:NH2	1:C:1478:ARG:HH11	1.78	0.81
1:F:3726:SER:CB	1:F:3729:ALA:HB2	2.10	0.81
1:B:941:ARG:H	1:D:2128:GLN:HE21	1.26	0.81
1:H:4848:CYS:HB2	1:H:4868:MET:CE	2.10	0.81
1:E:3341:ARG:H	1:G:4528:GLN:NE2	1.77	0.81
1:F:3713:THR:HG22	1:F:3842:SER:H	1.45	0.81
1:F:3941:ARG:H	1:H:5128:GLN:NE2	1.77	0.81
1:G:4477:ARG:NH2	1:G:4478:ARG:NH1	2.29	0.81
1:A:113:THR:CG2	1:A:242:SER:HB2	2.10	0.80
1:C:1313:THR:HG22	1:C:1442:SER:H	1.45	0.80
1:D:1824:THR:HG22	1:D:1827:GLU:CB	2.10	0.80
1:F:3731:VAL:HG12	1:F:3802:LEU:HB3	1.64	0.80
1:G:4276:SER:HB3	1:G:4319:ARG:HE	1.46	0.80
1:E:3493:MET:CE	1:E:3529:VAL:HG13	2.10	0.80
1:F:3648:CYS:HB2	1:F:3668:MET:CE	2.12	0.80
1:A:163:ILE:HG23	1:A:163:ILE:O	1.82	0.80
1:F:3624:THR:CG2	1:F:3627:GLU:H	1.93	0.80
1:F:3702:ILE:HG22	1:F:3703:LEU:HD12	1.63	0.80
1:A:69:ASN:HB3	1:A:463:HIS:ND1	1.97	0.80
1:B:759:ASP:HB3	6:B:6586:HOH:O	1.82	0.79
1:D:2176:MET:CE	1:D:2179:LEU:HB2	2.12	0.79
1:A:225:ILE:HG23	1:A:256:ILE:CG2	2.13	0.79
1:F:3740:LYS:HE2	1:F:3791:PHE:CD2	2.18	0.79
1:G:4680:ALA:HB3	1:G:4683:GLU:CG	2.13	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1472:ASN:ND2	1:C:1475:GLY:H	1.81	0.79
1:E:3191:PHE:HE2	1:E:3193:VAL:HG23	1.46	0.79
1:D:1899:SER:O	1:D:1901:PRO:HD3	1.83	0.79
1:B:650:ILE:HD11	1:B:668:MET:CE	2.11	0.79
1:D:2044:ILE:CG2	1:D:2082:ILE:HD12	2.13	0.79
1:D:1824:THR:CG2	1:D:1827:GLU:H	1.95	0.79
1:E:3431:THR:CG2	1:E:3434:GLY:HA2	2.12	0.79
1:C:1609:GLU:O	1:C:1613:MET:HG3	1.84	0.78
1:D:2304:LYS:HG3	1:D:2330:PRO:C	2.03	0.78
1:H:5327:VAL:HG13	1:H:5328:PRO:HD2	1.63	0.78
1:C:1259:THR:O	1:C:1263:MET:HG3	1.83	0.78
6:B:6064:HOH:O	1:D:1824:THR:HG21	1.84	0.78
1:A:126:SER:HB3	1:A:129:ALA:CB	2.12	0.78
1:H:4923:ILE:HD12	1:H:4931:VAL:HG23	1.66	0.78
1:A:511:LEU:HD22	1:A:521:THR:HG23	1.66	0.77
1:E:3465:TYR:HB2	1:E:3468:ILE:HD12	1.65	0.77
1:H:5209:GLU:O	1:H:5213:MET:HG3	1.84	0.77
1:F:3724:LYS:HG3	6:F:7409:HOH:O	1.85	0.77
1:G:4339:LEU:HD11	1:G:4354:ASN:CA	2.15	0.77
1:E:3253:VAL:HG12	1:E:3257:LEU:CD2	2.14	0.77
1:E:3225:ILE:HD12	1:E:3256:ILE:HD12	1.66	0.77
1:F:3787:LYS:HA	1:F:3792:LEU:HD12	1.67	0.77
1:A:277:ARG:NH2	1:A:278:ARG:NH1	2.33	0.77
1:A:515:ARG:HD2	6:A:6021:HOH:O	1.85	0.77
1:B:1104:LYS:HB3	1:B:1130:PRO:C	2.04	0.77
1:A:122:LEU:HD23	1:A:204:SER:CB	2.14	0.76
1:D:1902:ILE:HG13	1:D:2295:VAL:HG22	1.66	0.76
1:E:3479:GLU:HG3	6:E:6677:HOH:O	1.84	0.76
1:F:3949:ASN:HD21	1:H:5110:LYS:NZ	1.83	0.76
1:E:3246:LYS:HD2	1:E:3249:ASP:OD1	1.86	0.76
1:A:162:ASN:CB	1:A:162:ASN:N	2.49	0.76
1:E:3027:GLU:O	1:E:3031:ARG:HG3	1.86	0.76
1:C:1665:TYR:HB2	1:C:1668:ILE:HD12	1.67	0.76
1:E:3316:CYS:HB3	1:E:3321:LYS:O	1.84	0.76
1:A:328:GLN:HE21	1:C:1541:ARG:H	1.32	0.76
1:B:873:HIS:O	1:B:877:ARG:HG3	1.86	0.76
1:C:1409:ASN:O	1:C:1411:PRO:HD3	1.85	0.76
1:A:55:ARG:HD2	1:A:82:TYR:OH	1.84	0.76
1:H:5191:ARG:O	1:H:5195:GLU:HG3	1.84	0.76
1:B:976:MET:HE2	1:B:980:ILE:HD11	1.67	0.76
1:E:3172:LYS:HE3	1:E:3183:GLN:HB2	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4438:MET:HA	1:G:4464:ILE:HG23	1.66	0.76
1:G:4322:LEU:HD23	1:G:4404:SER:CB	2.15	0.76
1:G:4360:TYR:HE2	1:G:4366:VAL:HG21	1.51	0.76
1:B:1054:ARG:HD2	6:B:7369:HOH:O	1.85	0.76
1:G:4494:GLY:CA	1:G:4527:THR:HG21	2.17	0.75
1:A:221:SER:HB2	1:A:224:ASP:H	1.51	0.75
1:A:391:ARG:O	1:A:395:GLU:HG3	1.87	0.75
1:B:873:HIS:CE1	1:B:900:ILE:HG22	2.22	0.75
1:D:2201:SER:HA	1:D:2203:HIS:HE1	1.51	0.75
1:E:3493:MET:HE1	1:E:3529:VAL:HG13	1.67	0.75
1:C:1669:PHE:HB3	1:C:1699:ARG:NH1	2.01	0.75
1:F:3723:ILE:HA	1:F:3751:CYS:O	1.86	0.75
1:B:823:LYS:HE3	1:B:827:ASP:OD2	1.85	0.75
1:G:4250:ILE:HB	1:G:4273:MET:HE3	1.67	0.75
1:B:890:MET:HE2	1:B:892:ALA:HB2	1.68	0.75
1:G:4408:VAL:HG12	1:G:4410:LEU:CD1	2.17	0.74
1:B:740:LYS:HE2	1:B:742:THR:HG22	1.69	0.74
1:A:145:ASN:O	1:A:148:MET:HB2	1.87	0.74
1:C:1250:ILE:HD11	1:C:1268:MET:HE3	1.67	0.74
1:F:3732:GLU:HB2	1:F:3801:PHE:CD1	2.21	0.74
1:A:399:ARG:NH2	1:C:1223:ASP:HB2	2.03	0.74
1:G:4332:GLU:HA	1:G:4401:PHE:HA	1.69	0.74
1:H:5130:LEU:HD13	1:H:5133:MET:CE	2.16	0.74
1:A:122:LEU:HD12	1:A:149:GLU:HG2	1.67	0.74
1:H:5311:LEU:HB3	1:H:5321:THR:HG21	1.69	0.74
1:F:3652:PRO:HD2	1:F:3965:ALA:O	1.88	0.74
1:B:722:LEU:HA	1:B:804:SER:HB3	1.67	0.74
1:C:1678:GLN:CB	1:C:1684:ASP:HB2	2.15	0.74
1:B:866:ILE:O	1:B:887:ASP:HB2	1.88	0.74
1:C:1421:SER:O	1:C:1425:ILE:HG13	1.88	0.74
1:G:4368:ASP:O	1:G:4371:SER:HB2	1.87	0.74
1:A:192:LEU:N	1:A:192:LEU:HD22	2.02	0.74
1:C:1376:ASP:OD2	1:C:1406:LYS:HE2	1.87	0.74
1:H:4851:GLY:O	1:H:4855:ARG:HG2	1.86	0.74
1:A:48:CYS:HB2	1:A:68:MET:HE2	1.70	0.74
1:B:1125:ARG:HD2	6:B:7678:HOH:O	1.88	0.74
1:C:1345:ASN:O	1:C:1348:MET:HB3	1.86	0.74
1:C:1526:ALA:HB1	1:C:1559:MET:HE2	1.69	0.74
1:A:55:ARG:HD2	1:A:82:TYR:CZ	2.23	0.73
1:B:897:GLY:HA3	1:D:2141:ARG:HE	1.51	0.73
1:C:1313:THR:CG2	1:C:1442:SER:H	1.99	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:5108:ALA:O	1:H:5112:ILE:HG13	1.88	0.73
1:B:815:VAL:HB	1:B:817:LEU:CD1	2.18	0.73
1:B:941:ARG:H	1:D:2128:GLN:NE2	1.86	0.73
1:D:1817:LEU:O	1:D:1820:ALA:HB3	1.87	0.73
1:E:3252:GLU:O	1:E:3256:ILE:HG12	1.89	0.73
1:F:3648:CYS:HB2	1:F:3668:MET:HE2	1.68	0.73
1:A:147:TYR:HA	1:A:150:LYS:HB2	1.70	0.73
1:A:167:VAL:CG2	1:A:184:VAL:HG21	2.19	0.73
1:A:327:THR:HG22	1:A:328:GLN:HG3	1.69	0.73
1:C:1313:THR:HG22	1:C:1442:SER:OG	1.87	0.73
1:E:3392:LYS:O	1:E:3396:GLU:HG3	1.88	0.73
1:C:1363:ILE:O	1:C:1367:VAL:HG12	1.88	0.73
1:C:1428:LEU:HD13	1:C:1456:ILE:HB	1.71	0.73
1:C:1500:ILE:HB	1:C:1501:PRO:HD2	1.70	0.73
1:A:160:TYR:CD2	1:A:163:ILE:HB	2.19	0.73
1:B:1087:LEU:HD23	1:B:1088:ARG:N	2.04	0.73
1:G:4478:ARG:O	1:G:4482:ILE:HG13	1.89	0.73
1:B:928:GLN:NE2	1:D:2141:ARG:N	2.36	0.72
1:C:1286:THR:O	1:C:1290:VAL:HG23	1.89	0.72
1:C:1404:SER:O	1:C:1406:LYS:HD3	1.90	0.72
1:D:1848:CYS:HB2	1:D:1868:MET:CE	2.19	0.72
1:E:3493:MET:CE	1:E:3530:PRO:HD2	2.17	0.72
1:D:2284:ASP:O	1:D:2288:ARG:HG3	1.89	0.72
1:E:3426:ALA:HA	1:E:3447:ALA:HB1	1.70	0.72
1:B:950:ALA:O	1:B:953:ASP:HB2	1.89	0.72
1:C:1250:ILE:HB	1:C:1273:MET:CE	2.20	0.72
1:C:1526:ALA:HB1	1:C:1559:MET:CE	2.20	0.72
1:E:3172:LYS:HE2	1:E:3197:GLU:OE1	1.89	0.72
1:F:3999:ARG:HH12	1:H:4823:ASP:HB2	1.53	0.72
1:C:1291:ARG:O	1:C:1295:GLU:HG2	1.90	0.72
1:A:131:VAL:HG12	1:A:202:LEU:HD23	1.71	0.71
1:B:674:ASN:OD1	1:B:676:SER:HB2	1.90	0.71
1:D:2046:LYS:HB2	6:D:7775:HOH:O	1.90	0.71
1:F:3763:ILE:O	1:F:3767:VAL:HG13	1.91	0.71
1:A:118:ILE:HG22	1:A:208:VAL:HB	1.72	0.71
1:A:388:MET:HB2	1:A:390:HIS:CE1	2.24	0.71
1:C:1671:VAL:HG12	1:C:1691:LEU:HD21	1.72	0.71
1:A:485:VAL:O	1:A:489:VAL:HG23	1.89	0.71
1:C:1382:LEU:CD2	1:C:1396:VAL:HG22	2.21	0.71
1:C:1477:ARG:HH22	1:C:1478:ARG:NH1	1.88	0.71
1:D:1945:ASN:HD21	1:D:1961:LYS:NZ	1.88	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3188:GLY:HA3	1:E:3191:PHE:CE1	2.25	0.71
1:G:4591:ARG:NH1	1:G:4592:LYS:HD2	2.06	0.71
1:H:4963:ILE:O	1:H:4967:VAL:HG22	1.90	0.71
1:B:1111:LEU:HD21	1:B:1124:MET:HB2	1.71	0.71
1:D:1851:GLY:O	1:D:1855:ARG:HG3	1.91	0.71
1:G:4715:ARG:HB3	1:G:4716:PRO:HD2	1.71	0.71
1:A:288:GLY:O	1:A:289:ILE:HD13	1.89	0.71
1:C:1511:MET:O	1:C:1515:ARG:HG3	1.91	0.71
1:F:3776:ASP:OD2	1:F:3806:LYS:HE3	1.91	0.71
1:A:191:PHE:HE2	1:A:193:VAL:HG23	1.56	0.70
1:G:4509:GLN:O	1:G:4513:ILE:HG13	1.90	0.70
1:D:1855:ARG:HD2	1:D:1882:TYR:OH	1.90	0.70
1:A:496:GLY:HA3	1:A:502:PHE:CZ	2.26	0.70
1:D:1848:CYS:HB2	1:D:1868:MET:HE3	1.73	0.70
1:F:3752:ASP:OD1	1:F:3755:ILE:HD13	1.91	0.70
1:D:2044:ILE:HG13	1:D:2068:SER:HB3	1.72	0.70
1:D:2116:CYS:HB3	1:D:2121:LYS:O	1.91	0.70
1:A:506:ASP:O	1:A:529:VAL:HG23	1.92	0.70
1:C:1257:VAL:HG21	1:C:1292:THR:HG22	1.71	0.70
1:F:3669:ASN:HB3	1:F:4063:HIS:CD2	2.27	0.70
1:B:1091:LEU:O	1:B:1095:VAL:HG23	1.92	0.70
1:B:970:PRO:O	1:B:974:VAL:HG23	1.90	0.70
1:C:1322:LEU:HB2	1:C:1349:GLU:HA	1.72	0.70
1:G:4323:ILE:HD13	1:G:4351:CYS:HB3	1.73	0.70
1:F:3624:THR:HG22	1:F:3627:GLU:N	2.01	0.70
1:C:1327:GLY:HA2	1:C:1404:SER:CB	2.22	0.69
1:C:1319:ARG:H	1:C:1359:ASP:HB2	1.57	0.69
1:H:4966:VAL:HB	6:H:7456:HOH:O	1.91	0.69
1:H:5130:LEU:HD22	1:H:5133:MET:CE	2.22	0.69
1:A:246:LYS:HG3	6:A:7561:HOH:O	1.90	0.69
1:E:3160:TYR:CD2	1:E:3163:ILE:HB	2.26	0.69
1:D:1814:THR:HG22	1:D:1815:GLN:HG3	1.73	0.69
1:D:2188:MET:HE2	1:D:2266:ARG:HH21	1.57	0.69
1:G:4341:ILE:HB	1:G:4392:LEU:HB2	1.74	0.69
1:G:4445:ARG:O	1:G:4478:ARG:HD3	1.92	0.69
1:B:648:CYS:HB2	1:B:668:MET:HE3	1.74	0.69
1:C:1257:VAL:HG21	1:C:1292:THR:CG2	2.22	0.69
1:E:3493:MET:HE1	1:E:3529:VAL:HA	1.74	0.69
1:C:1459:GLU:O	1:C:1462:LYS:HG2	1.91	0.69
1:C:1493:ARG:HD3	1:C:1526:ALA:O	1.92	0.69
1:E:3411:MET:SD	1:F:4126:VAL:HG23	2.32	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4477:ARG:NH2	1:G:4478:ARG:HH11	1.89	0.69
1:G:4704:LYS:HG2	1:G:4730:PRO:C	2.12	0.69
1:C:1251:GLY:O	1:C:1255:ARG:HG3	1.91	0.69
1:E:3068:MET:HE1	1:E:3071:ALA:HB2	1.73	0.69
1:E:3478:GLN:HB2	1:E:3484:ASP:HB2	1.73	0.69
1:G:4216:GLN:HE22	1:G:4233:ASP:H	1.41	0.69
1:H:5314:TRP:CD1	1:H:5315:ARG:HG3	2.28	0.69
1:B:648:CYS:HB2	1:B:668:MET:HE2	1.75	0.69
1:F:3752:ASP:CG	1:F:3754:ASN:H	1.96	0.69
1:H:4952:ASP:HB2	1:H:4953:GLU:OE1	1.93	0.69
1:C:1501:PRO:HG2	1:C:1504:LYS:HD2	1.73	0.69
1:B:991:ARG:O	1:B:995:GLU:HG3	1.92	0.69
1:H:4942:THR:HG23	1:H:4944:ASP:N	2.04	0.69
1:A:328:GLN:HE22	1:C:1540:THR:HA	1.57	0.68
1:C:1723:THR:HG23	1:D:2325:ARG:HG3	1.73	0.68
1:F:3740:LYS:HE2	1:F:3791:PHE:CG	2.28	0.68
1:G:4257:VAL:O	1:G:4261:LYS:HG3	1.94	0.68
1:G:4408:VAL:HG12	1:G:4410:LEU:HD11	1.73	0.68
1:E:3432:GLU:HA	1:E:3432:GLU:OE1	1.92	0.68
1:G:4273:MET:HE3	1:G:4286:THR:HG21	1.75	0.68
1:G:4680:ALA:CB	1:G:4683:GLU:HG3	2.23	0.68
1:A:167:VAL:HG21	1:A:184:VAL:HG21	1.75	0.68
1:A:454:ARG:HG2	1:A:473:CYS:HB3	1.74	0.68
1:E:3222:GLU:HG2	1:E:3223:LYS:N	2.07	0.68
1:E:3475:ASP:HB3	1:E:3476:PRO:HD2	1.75	0.68
1:F:3743:LEU:HD11	1:F:3761:LYS:HA	1.76	0.68
1:C:1362:ASN:HD22	1:C:1365:LYS:HD2	1.59	0.68
1:D:2240:VAL:HG12	1:D:2249:ILE:CD1	2.23	0.68
1:A:225:ILE:HG23	1:A:256:ILE:HG23	1.75	0.68
1:D:2033:GLU:HG3	6:D:6665:HOH:O	1.93	0.68
1:F:3760:TYR:HE2	1:F:3766:VAL:HG21	1.58	0.68
1:B:1078:GLN:HA	1:B:1078:GLN:NE2	2.08	0.67
1:B:745:ASN:HD22	1:B:757:TRP:HE1	1.40	0.67
1:A:122:LEU:HB2	1:A:149:GLU:HA	1.75	0.67
1:E:3145:ASN:O	1:E:3148:MET:HB2	1.93	0.67
1:G:4293:ALA:O	1:G:4296:SER:HB3	1.95	0.67
1:A:481:TRP:O	1:A:485:VAL:HG23	1.95	0.67
1:C:1423:LYS:O	1:C:1426:GLN:HB3	1.95	0.67
1:A:310:LYS:NZ	1:C:1549:ASN:HD21	1.93	0.67
1:F:3845:ARG:HG2	1:F:3874:GLU:HB3	1.75	0.67
1:A:340:THR:OG1	1:A:343:GLU:HG3	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:GLN:HG3	1:A:39:ILE:HG23	1.75	0.67
1:B:716:PRO:HG2	1:B:843:PHE:CD2	2.29	0.67
1:B:999:ARG:HH12	1:D:1823:ASP:CB	2.06	0.67
1:E:3254:ARG:NH2	1:E:3287:ASP:OD2	2.28	0.67
1:G:4275:PHE:O	1:G:4314:LYS:HE3	1.94	0.67
1:C:1406:LYS:HE3	5:C:1735:ATP:O3'	1.95	0.67
1:B:844:ILE:HG13	1:B:868:SER:HB3	1.77	0.67
1:F:3650:ILE:HD11	1:F:3668:MET:HE2	1.76	0.67
1:G:4409:ASN:C	1:G:4410:LEU:HD12	2.15	0.67
1:A:99:SER:O	1:A:101:PRO:HD3	1.95	0.67
1:B:999:ARG:HH12	1:D:1823:ASP:HB2	1.60	0.67
1:C:1250:ILE:HD11	1:C:1268:MET:CE	2.24	0.67
1:D:1902:ILE:HG22	1:D:1903:LEU:CD2	2.25	0.67
1:D:2141:ARG:HG2	1:D:2141:ARG:HH11	1.59	0.67
1:D:2291:LEU:O	1:D:2295:VAL:HG23	1.95	0.67
1:E:3440:VAL:HG12	1:E:3449:ILE:HD11	1.75	0.67
1:F:3687:ILE:HD13	1:F:3709:VAL:HG11	1.75	0.67
1:F:3999:ARG:NH1	1:H:4823:ASP:HB2	2.10	0.67
1:H:5020:VAL:HG12	1:H:5021:SER:O	1.93	0.67
1:A:333:MET:CE	1:A:373:ALA:HA	2.25	0.67
1:C:1339:LEU:HD12	1:C:1340:LYS:H	1.60	0.67
1:C:1366:VAL:CG2	1:C:1413:ALA:HB1	2.25	0.67
1:F:3691:ARG:O	1:F:3695:GLU:HG2	1.94	0.67
1:F:3653:ALA:HB2	1:F:3966:LYS:HA	1.75	0.67
1:H:5020:VAL:CG1	1:H:5025:ILE:HG12	2.24	0.67
1:G:4360:TYR:CE2	1:G:4366:VAL:HG21	2.30	0.66
1:D:2090:MET:CE	1:D:2092:ALA:HB2	2.24	0.66
1:E:3481:TRP:HB2	1:E:3516:PRO:HG3	1.77	0.66
1:G:4665:TYR:CB	1:G:4668:ILE:HD12	2.23	0.66
1:H:4847:ILE:HG21	1:H:5159:MET:HE2	1.77	0.66
1:A:484:ASP:O	1:A:487:LEU:HB3	1.95	0.66
1:C:1362:ASN:ND2	1:C:1365:LYS:HD2	2.10	0.66
1:F:3684:ALA:HB2	1:F:3830:PHE:HZ	1.60	0.66
1:G:4477:ARG:HH22	1:G:4478:ARG:NH1	1.94	0.66
1:A:120:THR:HG22	1:A:205:LYS:H	1.60	0.66
1:A:84:ALA:HB2	1:A:230:PHE:HZ	1.61	0.66
1:B:1111:LEU:CD2	1:B:1124:MET:HB2	2.26	0.66
1:C:1370:GLY:O	1:C:1383:GLN:NE2	2.29	0.66
1:H:5130:LEU:HD22	1:H:5133:MET:HE3	1.77	0.66
1:A:203:GLY:HA3	1:A:206:LYS:HE2	1.76	0.66
1:A:292:ALA:HB1	3:A:533:OXL:C1	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:827:ASP:O	1:B:830:PHE:HB3	1.94	0.66
1:C:1387:LYS:HB3	1:C:1392:LEU:HD12	1.78	0.66
1:E:3448:PRO:HB3	1:E:3469:PHE:CE1	2.31	0.66
1:H:5311:LEU:HB3	1:H:5321:THR:HG23	1.75	0.66
1:C:1323:ILE:HG22	1:C:1324:LYS:HG3	1.76	0.66
1:C:1343:LEU:HD13	1:C:1390:ASP:O	1.96	0.66
1:B:938:ARG:HH22	1:D:1998:ASN:HD21	1.43	0.66
1:E:3509:ILE:CD1	1:E:3526:VAL:HG23	2.25	0.66
1:G:4342:THR:HG21	1:G:4347:TYR:CD2	2.31	0.66
1:G:4493:ARG:HD3	1:G:4526:ALA:O	1.95	0.66
1:B:768:ASP:O	1:B:771:SER:HB2	1.95	0.66
1:C:1441:ALA:O	1:C:1469:LYS:HG3	1.95	0.66
1:D:1941:ILE:HA	1:D:1956:LEU:O	1.96	0.66
1:D:2030:PHE:CE1	1:D:2034:GLN:HG3	2.31	0.66
1:H:4847:ILE:HB	1:H:5159:MET:HE3	1.78	0.66
1:F:3904:LYS:HD3	1:H:5183:GLU:OE2	1.96	0.66
1:B:651:GLY:O	1:B:655:ARG:HG3	1.97	0.65
1:C:1456:ILE:HD13	1:C:1456:ILE:N	2.11	0.65
1:A:173:VAL:HG13	1:A:210:LEU:HD11	1.77	0.65
1:B:866:ILE:C	1:B:867:ILE:HD13	2.17	0.65
1:C:1326:SER:HB3	1:C:1329:ALA:CB	2.26	0.65
1:C:1343:LEU:HD23	1:C:1361:LYS:CD	2.25	0.65
1:C:1313:THR:HG21	6:C:6155:HOH:O	1.95	0.65
1:D:2171:LEU:O	1:D:2175:ARG:HG3	1.96	0.65
1:E:3457:GLN:O	1:E:3461:GLN:HG3	1.96	0.65
1:A:333:MET:HG2	1:A:336:LYS:O	1.96	0.65
1:C:1581:ALA:O	1:C:1585:GLU:HG3	1.96	0.65
1:D:2072:ASN:HB2	6:D:6547:HOH:O	1.96	0.65
1:F:3757:TRP:C	1:F:3758:LEU:HD23	2.17	0.65
1:C:1366:VAL:HG22	1:C:1413:ALA:HB1	1.77	0.65
1:E:3160:TYR:HD2	1:E:3163:ILE:CB	2.09	0.65
1:G:4250:ILE:HB	1:G:4273:MET:CE	2.27	0.65
1:G:4498:ILE:N	1:G:4498:ILE:HD13	2.11	0.65
1:G:4555:ALA:O	1:G:4666:ARG:NH1	2.29	0.65
1:H:5066:ILE:C	1:H:5067:ILE:HD13	2.17	0.65
1:C:1531:GLU:N	1:C:1543:GLU:OE2	2.30	0.65
1:A:14:THR:HG23	1:A:15:GLN:HB2	1.77	0.65
1:G:4321:GLY:HA3	1:G:4357:TRP:HE3	1.62	0.65
1:A:103:LEU:HD11	1:A:498:ALA:HB1	1.78	0.65
1:E:3371:LEU:HB2	6:E:6190:HOH:O	1.97	0.65
1:A:160:TYR:O	1:A:163:ILE:HG22	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:MET:SD	1:B:1021:LYS:HD3	2.37	0.65
1:D:2241:ALA:O	1:D:2244:ARG:NH1	2.29	0.65
5:A:535:ATP:N7	6:A:7651:HOH:O	2.30	0.65
1:C:1427:ASP:O	1:C:1430:PHE:HB3	1.97	0.65
1:C:1477:ARG:HH22	1:C:1478:ARG:HH11	1.44	0.65
1:D:2265:TYR:HB2	1:D:2268:ILE:CD1	2.26	0.65
1:C:1442:SER:CA	1:C:1469:LYS:HD3	2.26	0.64
1:G:4247:ILE:HB	1:G:4559:MET:HG3	1.78	0.64
1:A:73:MET:HE2	1:A:86:THR:HG21	1.79	0.64
1:B:934:ILE:HG23	1:B:967:GLY:HA2	1.80	0.64
1:B:969:TYR:HB3	1:B:972:GLU:HB2	1.79	0.64
1:D:2176:MET:HE3	1:D:2179:LEU:HB2	1.77	0.64
1:H:5015:VAL:CG1	1:H:5017:LEU:HG	2.28	0.64
1:B:1031:THR:HG21	1:B:1034:GLY:HA2	1.78	0.64
1:C:1273:MET:HE2	1:C:1286:THR:HG21	1.80	0.64
1:C:1479:PHE:HE1	1:C:1489:ILE:HD12	1.60	0.64
1:E:3315:ARG:NH1	1:G:4230:CYS:O	2.29	0.64
1:F:3838:MET:HA	1:F:3864:ILE:HG23	1.79	0.64
1:A:246:LYS:HG3	1:A:248:ALA:HB3	1.80	0.64
1:A:57:VAL:HG22	1:A:89:ASN:HA	1.78	0.64
1:F:3731:VAL:O	1:F:3802:LEU:N	2.30	0.64
1:G:4348:MET:HA	1:G:4357:TRP:CD2	2.33	0.64
1:G:4410:LEU:O	1:G:4413:ALA:HB3	1.98	0.64
1:A:50:ILE:HB	1:A:73:MET:CE	2.26	0.64
1:C:1319:ARG:NE	1:C:1405:LYS:O	2.30	0.64
1:E:3288:GLY:C	1:E:3289:ILE:HG12	2.17	0.64
1:E:3376:MET:HE2	1:E:3380:ILE:HG13	1.80	0.64
1:E:3481:TRP:CG	1:E:3516:PRO:HD3	2.33	0.64
1:F:3787:LYS:HB3	1:F:3792:LEU:CD1	2.27	0.64
1:F:3788:GLY:N	1:F:3791:PHE:O	2.29	0.64
1:G:4374:TYR:HB3	1:G:4378:GLY:HA2	1.79	0.64
1:C:1360:TYR:HE2	1:C:1366:VAL:HG11	1.61	0.64
1:D:1855:ARG:NH2	1:D:1885:GLU:HG2	2.11	0.64
1:A:399:ARG:HD2	6:C:6738:HOH:O	1.98	0.64
1:F:3713:THR:CG2	1:F:3842:SER:H	2.09	0.64
1:G:4389:PRO:HD2	1:G:4391:PHE:HE2	1.63	0.64
1:B:867:ILE:HD13	1:B:867:ILE:N	2.13	0.64
1:E:3051:GLY:O	1:E:3055:ARG:HG3	1.97	0.64
1:F:3612:ILE:N	6:F:7416:HOH:O	2.29	0.64
1:H:5020:VAL:HG13	1:H:5024:ASP:CB	2.26	0.63
1:A:269:LYS:HE3	1:A:290:MET:HE1	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1910:ALA:HB2	1:D:2038:MET:HG3	1.80	0.63
1:F:3698:ALA:HB2	1:F:3704:TYR:CD1	2.34	0.63
1:H:5067:ILE:HD13	1:H:5067:ILE:N	2.12	0.63
1:A:486:ASP:O	1:A:490:ASN:ND2	2.29	0.63
1:C:1530:LEU:O	1:C:1563:GLU:HG2	1.98	0.63
1:F:3688:LYS:HE3	6:F:7588:HOH:O	1.97	0.63
1:F:3722:LEU:O	1:F:3751:CYS:N	2.28	0.63
1:A:131:VAL:CG1	1:A:202:LEU:HD23	2.28	0.63
1:A:164:CYS:O	1:A:187:LYS:NZ	2.31	0.63
1:D:2054:ARG:NH2	1:D:2062:LYS:O	2.31	0.63
1:G:4339:LEU:HD11	1:G:4354:ASN:HA	1.79	0.63
1:C:1343:LEU:HD23	1:C:1361:LYS:HD2	1.80	0.63
1:F:3976:MET:O	1:F:3980:ILE:HG13	1.98	0.63
1:G:4493:ARG:HH12	1:G:4529:MET:HG2	1.61	0.63
1:B:871:GLU:HG2	1:B:892:ALA:HB3	1.79	0.63
1:G:4322:LEU:O	1:G:4351:CYS:HB2	1.98	0.63
1:A:130:GLU:HA	1:A:202:LEU:O	1.99	0.63
1:C:1255:ARG:HD2	1:C:1282:TYR:CZ	2.33	0.63
1:D:2245:PRO:HD2	6:D:6576:HOH:O	1.99	0.63
1:E:3012:ILE:HG22	1:E:3013:GLN:N	2.14	0.63
1:C:1509:GLN:HG2	1:C:1513:ILE:HD12	1.80	0.63
1:A:310:LYS:HZ1	1:C:1549:ASN:HD21	1.47	0.63
1:F:3650:ILE:HD11	1:F:3668:MET:CE	2.29	0.63
1:F:3679:THR:OG1	1:F:3680:HIS:N	2.29	0.63
1:A:280:ASP:OD1	1:A:315:ARG:NH1	2.32	0.63
1:A:421:LYS:HE2	1:B:1013:MET:SD	2.38	0.63
1:D:1860:LEU:O	1:D:1864:ILE:HG13	1.99	0.63
1:D:2190:HIS:CD2	1:D:2246:ARG:HG3	2.34	0.63
1:E:3099:SER:O	1:E:3101:PRO:HD3	1.98	0.63
1:E:3220:VAL:HG11	1:E:3225:ILE:CD1	2.29	0.63
1:H:4815:GLN:HG3	1:H:4839:ILE:HG23	1.81	0.63
1:G:4704:LYS:HE2	1:G:4730:PRO:O	1.98	0.62
1:A:57:VAL:HG22	1:A:89:ASN:CA	2.28	0.62
1:B:1099:ARG:HB3	1:B:1101:PHE:CE1	2.34	0.62
1:F:4075:ASP:CB	1:F:4087:LEU:HD21	2.30	0.62
1:G:4322:LEU:CD2	1:G:4327:GLY:HA2	2.29	0.62
1:A:231:GLY:O	1:A:236:VAL:HG13	1.98	0.62
1:B:649:THR:OG1	1:B:672:ARG:NH1	2.30	0.62
1:F:3828:LEU:O	1:F:3832:VAL:HG23	1.99	0.62
1:A:522:ASN:H	1:A:522:ASN:HD22	1.45	0.62
1:E:3333:MET:HA	1:E:3336:LYS:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3355:ALA:O	1:E:3466:ARG:NH1	2.31	0.62
1:F:4113:GLY:HA2	1:F:4122:ASN:OD1	1.99	0.62
1:G:4508:ALA:O	1:G:4512:ILE:HG13	1.98	0.62
1:E:3328:GLN:HE21	1:G:4540:THR:HB	1.63	0.62
1:H:5133:MET:CE	1:H:5139:PRO:HB3	2.29	0.62
1:H:4945:ASN:HB3	1:H:4948:MET:HE2	1.80	0.62
1:A:123:ILE:HD11	1:A:202:LEU:HG	1.81	0.62
1:C:1319:ARG:NH2	5:C:1735:ATP:O1B	2.33	0.62
1:C:1360:TYR:HD2	1:C:1363:ILE:HB	1.64	0.62
1:C:1675:ASP:HB3	1:C:1676:PRO:HD2	1.81	0.62
1:E:3372:GLU:OE1	1:E:3372:GLU:N	2.30	0.62
1:C:1339:LEU:HD12	1:C:1340:LYS:N	2.15	0.62
1:D:1814:THR:HG23	1:D:1837:ALA:O	1.98	0.62
1:F:3655:ARG:HD2	1:F:3682:TYR:OH	2.00	0.62
1:H:4876:SER:HA	1:H:4914:LYS:HG3	1.82	0.62
1:C:1633:SER:OG	1:C:1635:ARG:HG3	1.99	0.62
1:E:3330:LEU:HD12	1:E:3343:GLU:HB3	1.81	0.62
1:F:3750:LYS:O	1:F:3755:ILE:HD11	1.99	0.62
1:F:3825:ILE:O	1:F:3829:LYS:HG2	2.00	0.62
1:A:120:THR:HG22	1:A:205:LYS:N	2.15	0.61
1:B:658:GLU:HG3	6:B:7721:HOH:O	1.99	0.61
1:B:748:MET:HB2	1:B:757:TRP:CE2	2.35	0.61
1:F:3856:ILE:N	1:F:3856:ILE:HD13	2.13	0.61
1:F:3966:LYS:HG2	1:F:3966:LYS:O	1.98	0.61
1:D:1863:MET:HG2	1:D:2171:LEU:HD23	1.81	0.61
1:H:4932:GLU:HG3	1:H:5001:PHE:CE1	2.36	0.61
1:A:223:LYS:O	1:A:226:GLN:HB2	1.99	0.61
1:C:1429:LYS:O	1:C:1433:GLU:HG2	2.00	0.61
1:B:650:ILE:N	1:B:650:ILE:HD13	2.16	0.61
6:A:7271:HOH:O	1:C:1542:ALA:HB3	1.99	0.61
1:G:4384:VAL:HA	1:G:4394:THR:HG22	1.82	0.61
1:G:4527:THR:OG1	3:G:4733:OXL:O2	2.15	0.61
1:A:108:ALA:HB2	1:A:460:ARG:HB3	1.82	0.61
1:C:1591:ARG:NH1	1:C:1592:LYS:HE3	2.15	0.61
1:D:1919:ARG:H	1:D:1959:ASP:HB2	1.66	0.61
1:D:2226:ALA:HA	1:D:2247:ALA:HB1	1.83	0.61
1:G:4367:VAL:CG2	1:G:4371:SER:HB3	2.26	0.61
1:B:654:SER:O	1:B:660:LEU:HD13	1.99	0.61
1:B:720:THR:HA	1:B:758:LEU:HD23	1.83	0.61
1:C:1532:SER:HB2	1:C:1543:GLU:OE1	2.00	0.61
1:C:1657:GLN:O	1:C:1661:GLN:HG3	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1678:GLN:HA	1:C:1678:GLN:NE2	2.15	0.61
1:F:3760:TYR:CE2	1:F:3766:VAL:HG21	2.36	0.61
1:G:4253:ALA:HB2	1:G:4566:LYS:HA	1.81	0.61
1:A:188:GLY:HA3	1:A:191:PHE:CE1	2.35	0.61
1:F:3758:LEU:HD23	1:F:3758:LEU:N	2.16	0.61
1:G:4243:ASN:HB3	1:G:4667:GLY:CA	2.31	0.61
1:G:4300:ASP:OD2	1:G:4303:LEU:HB2	1.99	0.61
1:A:113:THR:HG22	1:A:242:SER:CB	2.23	0.61
1:C:1341:ILE:HD12	1:C:1394:THR:HG21	1.81	0.61
1:D:2044:ILE:HG22	1:D:2082:ILE:CD1	2.26	0.61
1:E:3452:VAL:HG11	1:E:3488:ARG:HB3	1.83	0.61
1:F:4008:MET:HG3	1:F:4039:GLN:HG2	1.83	0.61
1:G:4703:LYS:O	1:G:4729:VAL:HB	2.01	0.61
1:E:3220:VAL:HG11	1:E:3225:ILE:HD13	1.83	0.61
1:H:4850:ILE:N	1:H:4850:ILE:HD13	2.16	0.61
1:A:173:VAL:HG13	1:A:210:LEU:CD1	2.31	0.61
1:C:1378:GLY:HA3	1:C:1498:ILE:HG13	1.83	0.61
1:F:3892:ALA:HB1	3:F:4133:OXL:C2	2.31	0.60
1:G:4388:GLY:HA3	1:G:4391:PHE:CE2	2.36	0.60
1:A:141:ILE:HG21	1:A:158:LEU:CD2	2.24	0.60
1:C:1255:ARG:HD2	1:C:1282:TYR:OH	2.01	0.60
1:C:1385:LYS:HB2	1:C:1393:VAL:O	2.01	0.60
1:D:2240:VAL:HG12	1:D:2249:ILE:HD13	1.83	0.60
1:F:3890:MET:HE1	1:F:3892:ALA:HB2	1.83	0.60
1:A:133:LEU:N	1:A:133:LEU:HD13	2.16	0.60
1:B:989:PHE:CE2	1:B:992:LYS:HD2	2.36	0.60
1:B:1091:LEU:O	1:B:1091:LEU:HD12	2.01	0.60
1:C:1522:PRO:HA	1:C:1556:ASP:OD2	2.00	0.60
1:E:3113:THR:HG21	6:E:6221:HOH:O	2.00	0.60
1:F:3661:LYS:O	1:F:3665:LYS:HG3	2.00	0.60
1:C:1715:ARG:HB3	1:C:1716:PRO:HD2	1.83	0.60
1:E:3122:LEU:HB2	1:E:3149:GLU:HA	1.83	0.60
1:E:3506:ASP:O	1:E:3529:VAL:HG23	2.01	0.60
1:F:3702:ILE:HG22	1:F:3703:LEU:CD1	2.31	0.60
1:A:49:THR:OG1	1:A:72:ARG:HD3	2.02	0.60
1:B:1115:ARG:HB3	1:B:1116:PRO:CD	2.32	0.60
1:B:619:ALA:HA	1:B:631:ARG:HD2	1.83	0.60
1:C:1327:GLY:HA2	1:C:1404:SER:HB2	1.84	0.60
1:F:3903:GLU:OE1	1:F:3903:GLU:N	2.29	0.60
1:G:4471:GLU:OE1	1:G:4495:ASP:HB2	2.01	0.60
1:A:301:PRO:HG2	1:A:304:LYS:CD	2.30	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:3786:GLN:O	1:F:3793:VAL:N	2.28	0.60
1:F:4075:ASP:HB3	1:F:4076:PRO:HD2	1.84	0.60
1:G:4313:THR:HG21	6:G:6257:HOH:O	2.02	0.60
1:A:47:ILE:CG2	1:A:359:MET:HG3	2.31	0.60
1:B:1065:TYR:CB	1:B:1068:ILE:HD12	2.30	0.60
1:C:1257:VAL:CG2	1:C:1292:THR:HG22	2.31	0.60
1:E:3160:TYR:HE2	1:E:3166:VAL:HG21	1.67	0.60
1:A:237:ASP:OD1	1:A:460:ARG:NH1	2.34	0.60
1:F:3655:ARG:HD2	1:F:3682:TYR:CZ	2.37	0.60
1:G:4323:ILE:H	1:G:4404:SER:HB3	1.67	0.60
1:C:1728:PRO:O	1:C:1730:PRO:HD3	2.02	0.59
1:H:4855:ARG:NH2	1:H:4885:GLU:HB3	2.17	0.59
1:F:3928:GLN:NE2	1:H:5140:THR:HB	2.17	0.59
1:B:990:HIS:CD2	1:B:990:HIS:H	2.20	0.59
1:C:1493:ARG:NH1	1:C:1527:THR:O	2.36	0.59
1:D:2315:ARG:HB3	1:D:2316:PRO:HD2	1.84	0.59
1:E:3339:PRO:HG3	1:E:3376:MET:HG2	1.84	0.59
1:G:4492:ALA:HB1	3:G:4733:OXL:C2	2.32	0.59
1:E:3237:ASP:OD1	1:E:3460:ARG:HD2	2.02	0.59
1:A:225:ILE:HG23	1:A:256:ILE:HG21	1.83	0.59
1:F:3928:GLN:HE22	1:H:5140:THR:HA	1.68	0.59
1:G:4255:ARG:HD2	1:G:4282:TYR:OH	2.02	0.59
1:G:4409:ASN:C	1:G:4411:PRO:HD3	2.22	0.59
1:C:1713:GLY:HA2	1:C:1722:ASN:OD1	2.03	0.59
1:D:2045:ARG:C	1:D:2046:LYS:HG3	2.22	0.59
1:D:2083:LEU:O	1:D:2121:LYS:NZ	2.34	0.59
1:F:3752:ASP:OD2	1:F:3754:ASN:HB2	2.02	0.59
1:A:293:ARG:O	1:C:1541:ARG:NE	2.31	0.59
1:C:1341:ILE:HB	1:C:1392:LEU:HB2	1.83	0.59
1:D:1857:VAL:O	1:D:1861:LYS:HG3	2.02	0.59
1:E:3328:GLN:HE22	1:G:4540:THR:HA	1.67	0.59
1:F:3722:LEU:HD12	1:F:3749:GLU:OE1	2.03	0.59
1:G:4493:ARG:NH2	1:G:4546:ASP:OD1	2.35	0.59
1:B:639:ILE:O	1:B:982:ARG:HD2	2.03	0.59
1:D:1902:ILE:HG22	1:D:1903:LEU:HD21	1.83	0.59
1:E:3341:ARG:N	1:G:4528:GLN:NE2	2.47	0.59
1:G:4333:LEU:HG	1:G:4402:LEU:HD23	1.83	0.59
1:G:4681:TRP:CD2	1:G:4716:PRO:HD3	2.38	0.59
1:C:1491:VAL:HG23	1:C:1524:ILE:O	2.03	0.59
1:D:1850:ILE:HG13	1:D:1873:MET:HE1	1.85	0.59
1:E:3481:TRP:CD1	1:E:3516:PRO:HD3	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:3726:SER:HB3	1:F:3729:ALA:CB	2.30	0.59
1:F:3872:ASN:HD22	1:F:3875:GLY:H	1.50	0.59
1:G:4348:MET:HG2	1:G:4357:TRP:CZ2	2.37	0.59
1:G:4479:PHE:HZ	1:G:4483:LEU:HD22	1.67	0.59
1:G:4467:ILE:HD12	1:G:4488:GLY:HA3	1.84	0.59
1:G:4681:TRP:CG	1:G:4716:PRO:HD3	2.38	0.59
1:H:5281:TRP:CG	1:H:5316:PRO:HD3	2.37	0.59
1:B:886:SER:O	1:B:921:LYS:HE2	2.03	0.58
1:E:3433:SER:OG	1:E:3435:ARG:HB3	2.03	0.58
1:F:3719:ARG:O	1:F:3759:ASP:HB2	2.02	0.58
1:G:4654:ARG:HD2	6:G:6523:HOH:O	2.03	0.58
1:H:5106:PHE:O	1:H:5110:LYS:HG3	2.02	0.58
1:A:134:LYS:O	1:A:196:VAL:HB	2.03	0.58
1:A:268:SER:HB2	1:A:289:ILE:CD1	2.33	0.58
1:B:764:CYS:O	1:B:787:LYS:NZ	2.29	0.58
1:A:341:ARG:NE	1:C:1493:ARG:O	2.30	0.58
1:F:3742:THR:N	1:F:3756:LEU:O	2.31	0.58
1:F:3859:GLU:O	1:F:3862:LYS:HG3	2.04	0.58
1:E:3421:LYS:HD3	1:F:4013:MET:SD	2.43	0.58
1:G:4339:LEU:HD11	1:G:4354:ASN:C	2.22	0.58
1:A:141:ILE:HA	1:A:156:LEU:O	2.03	0.58
1:A:73:MET:CE	1:A:86:THR:HG21	2.34	0.58
1:A:407:LEU:HD21	1:B:1107:VAL:HG21	1.84	0.58
1:E:3172:LYS:HE2	1:E:3197:GLU:CD	2.23	0.58
1:D:2122:PRO:HG3	1:D:2265:TYR:CE2	2.38	0.58
1:E:3142:THR:HG22	1:E:3143:LEU:N	2.19	0.58
1:F:3717:GLU:OE2	1:F:3719:ARG:NH2	2.35	0.58
1:F:3928:GLN:NE2	1:H:5141:ARG:N	2.49	0.58
1:G:4477:ARG:HH21	1:G:4478:ARG:HH11	1.51	0.58
1:C:1360:TYR:HE2	1:C:1366:VAL:CG1	2.15	0.58
1:E:3376:MET:HE3	1:E:3379:LEU:HB2	1.85	0.58
1:F:3715:GLY:O	1:F:3717:GLU:N	2.36	0.58
1:H:5275:ASP:HB3	1:H:5276:PRO:HD2	1.85	0.58
1:C:1453:VAL:HG12	1:C:1457:LEU:HD22	1.86	0.58
1:D:2176:MET:HE3	1:D:2176:MET:CA	2.29	0.58
1:G:4383:GLN:O	1:G:4394:THR:HG22	2.04	0.58
1:E:3328:GLN:NE2	1:G:4540:THR:HB	2.18	0.58
1:H:4852:PRO:HD2	1:H:5165:ALA:O	2.04	0.58
1:A:141:ILE:N	1:A:192:LEU:O	2.30	0.58
1:B:673:MET:CE	1:B:686:THR:HG22	2.34	0.58
1:D:1855:ARG:HD3	6:D:7309:HOH:O	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:3726:SER:HB2	1:F:3729:ALA:HB2	1.85	0.58
1:G:4498:ILE:HD13	1:G:4498:ILE:H	1.69	0.58
1:H:5311:LEU:HD22	1:H:5321:THR:HG23	1.86	0.58
1:A:333:MET:HE1	1:A:373:ALA:HA	1.84	0.58
1:A:511:LEU:CD2	1:A:521:THR:HG23	2.34	0.58
1:B:658:GLU:HG2	6:B:7720:HOH:O	2.04	0.58
1:C:1326:SER:HB3	1:C:1329:ALA:HB2	1.86	0.58
1:E:3016:GLN:NE2	6:E:6183:HOH:O	2.36	0.58
1:G:4494:GLY:N	1:G:4527:THR:HG21	2.18	0.58
1:D:1873:MET:HE2	1:D:1886:THR:HG22	1.84	0.58
1:G:4251:GLY:O	1:G:4255:ARG:HG3	2.04	0.58
1:A:329:MET:O	1:A:343:GLU:HB3	2.04	0.57
1:B:731:VAL:O	1:B:801:PHE:HA	2.04	0.57
1:C:1347:TYR:HD2	1:C:1355:ILE:HG21	1.65	0.57
1:C:1422:GLU:O	1:C:1425:ILE:HB	2.04	0.57
1:C:1478:ARG:O	1:C:1482:ILE:HG13	2.04	0.57
1:E:3019:ALA:HB2	1:E:3031:ARG:HB2	1.86	0.57
1:F:4085:VAL:O	1:F:4089:VAL:HG23	2.04	0.57
1:G:4302:ILE:HD12	1:G:4694:ASN:CB	2.33	0.57
1:A:49:THR:HG22	1:A:365:ALA:HB2	1.84	0.57
1:A:506:ASP:C	1:A:529:VAL:HG23	2.25	0.57
1:C:1714:TRP:HD1	1:C:1715:ARG:HE	1.53	0.57
1:E:3191:PHE:C	1:E:3192:LEU:HD22	2.23	0.57
1:G:4391:PHE:HE1	1:G:4393:VAL:HG23	1.69	0.57
1:G:4493:ARG:HH22	1:G:4546:ASP:CG	2.08	0.57
1:H:5038:MET:CE	1:H:5264:LEU:HD22	2.34	0.57
1:A:290:MET:HG3	1:A:324:ILE:HB	1.86	0.57
1:B:745:ASN:ND2	1:B:757:TRP:HE1	2.02	0.57
1:E:3376:MET:CE	1:E:3376:MET:HA	2.31	0.57
1:H:4967:VAL:O	1:H:4987:LYS:NZ	2.36	0.57
1:A:514:TRP:H	1:A:522:ASN:ND2	1.92	0.57
1:E:3142:THR:HG21	1:E:3144:ASP:HB3	1.85	0.57
1:F:3660:LEU:HD13	1:F:3690:VAL:HA	1.87	0.57
1:A:172:LYS:HE3	1:A:197:GLU:OE2	2.04	0.57
1:B:1028:ILE:HD13	1:B:1092:ALA:CB	2.34	0.57
1:B:716:PRO:HG2	1:B:843:PHE:HB3	1.87	0.57
1:C:1714:TRP:CE3	1:D:2325:ARG:HD3	2.39	0.57
1:C:1533:MET:HA	1:C:1536:LYS:O	2.04	0.57
1:D:2093:ARG:HD3	1:D:2126:ALA:O	2.05	0.57
1:E:3316:CYS:O	1:E:3320:GLY:N	2.36	0.57
1:E:3390:HIS:HD2	6:E:6368:HOH:O	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:5130:LEU:HB3	1:H:5133:MET:HE3	1.86	0.57
1:H:5314:TRP:O	1:H:5315:ARG:HG2	2.05	0.57
1:A:399:ARG:NH2	1:C:1223:ASP:OD2	2.38	0.57
1:G:4274:ASN:HA	1:G:4312:ASP:HB3	1.87	0.57
1:A:518:SER:HB2	6:A:7635:HOH:O	2.05	0.57
1:C:1378:GLY:CA	1:C:1498:ILE:HG13	2.34	0.57
1:D:1887:ILE:N	1:D:1887:ILE:HD13	2.19	0.57
1:E:3144:ASP:HB3	1:E:3147:TYR:HD2	1.70	0.57
1:G:4457:LEU:HD12	1:G:4466:ILE:HD11	1.85	0.57
1:G:4666:ARG:HG3	1:G:4667:GLY:N	2.19	0.57
1:B:740:LYS:HE2	1:B:742:THR:CG2	2.35	0.57
1:C:1318:ILE:CG2	1:C:1408:VAL:HB	2.35	0.57
1:C:1537:PRO:HG2	1:C:1538:ARG:NH2	2.19	0.57
1:D:1842:ARG:NH1	1:D:1846:ILE:HG13	2.19	0.57
1:E:3440:VAL:HG12	1:E:3449:ILE:CD1	2.35	0.57
1:H:5133:MET:HE2	1:H:5139:PRO:CB	2.35	0.57
1:A:191:PHE:CE2	1:A:193:VAL:HG23	2.38	0.57
1:B:971:LEU:O	1:B:975:ARG:HD2	2.04	0.57
1:D:1855:ARG:NH2	1:D:1885:GLU:HB3	2.20	0.57
1:E:3041:ALA:HB2	1:E:3501:PHE:CE1	2.39	0.57
1:E:3160:TYR:CE2	1:E:3162:ASN:HB3	2.40	0.57
1:F:3648:CYS:HB2	1:F:3668:MET:HE3	1.85	0.57
1:F:3723:ILE:HG12	1:F:3804:SER:OG	2.05	0.57
1:A:133:LEU:N	1:A:200:GLY:O	2.35	0.56
1:D:1958:LEU:HD21	1:D:2008:VAL:HG21	1.87	0.56
1:G:4302:ILE:HD12	1:G:4694:ASN:HB2	1.85	0.56
1:A:144:ASP:HB3	1:A:147:TYR:HD1	1.70	0.56
1:A:503:LYS:O	1:A:506:ASP:HB2	2.05	0.56
1:A:86:THR:HG22	1:A:87:ILE:N	2.20	0.56
1:B:1057:GLN:O	1:B:1061:GLN:HG3	2.05	0.56
1:F:3739:LEU:HD21	1:F:3756:LEU:HB2	1.87	0.56
1:G:4336:GLY:N	1:G:4396:VAL:O	2.37	0.56
1:B:1127:VAL:HG12	1:B:1128:PRO:N	2.20	0.56
1:B:869:LYS:HE3	1:B:890:MET:HE1	1.87	0.56
1:C:1452:GLU:O	1:C:1455:LYS:HB3	2.04	0.56
1:G:4408:VAL:CG1	1:G:4410:LEU:HD11	2.35	0.56
1:D:1910:ALA:HB2	1:D:2038:MET:CG	2.35	0.56
3:F:4133:OXL:O1	6:F:6293:HOH:O	2.17	0.56
1:A:375:ARG:O	1:A:378:HIS:HB3	2.06	0.56
1:D:1952:ASP:OD1	1:D:1955:ILE:N	2.35	0.56
1:E:3091:ARG:O	1:E:3095:GLU:HG2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3198:ASN:ND2	6:E:6391:HOH:O	2.37	0.56
1:E:3272:ASN:OD1	1:E:3274:GLU:HB3	2.05	0.56
1:F:3711:LEU:O	1:F:3711:LEU:HD23	2.05	0.56
1:H:4920:THR:HB	1:H:4956:LEU:HD11	1.87	0.56
1:A:351:VAL:O	1:A:466:ARG:NH2	2.37	0.56
1:A:48:CYS:CB	1:A:68:MET:HE2	2.35	0.56
1:E:3230:PHE:CE1	1:E:3234:GLN:HG3	2.40	0.56
1:E:3245:ARG:CB	1:E:3274:GLU:HG2	2.30	0.56
1:E:3276:VAL:HG11	1:G:4234:ILE:HD13	1.86	0.56
1:G:4344:ASP:OD1	1:G:4346:ALA:HB3	2.04	0.56
1:A:18:HIS:O	1:A:21:MET:HB2	2.06	0.56
1:C:1363:ILE:HA	1:C:1366:VAL:HG12	1.86	0.56
1:C:1471:GLU:HB2	1:C:1495:ASP:HB2	1.88	0.56
1:G:4358:LEU:HD21	1:G:4363:ILE:HD12	1.88	0.56
1:G:4630:LEU:HD12	1:G:4712:THR:HG22	1.87	0.56
1:A:328:GLN:NE2	1:C:1541:ARG:N	2.50	0.56
1:A:435:ARG:HA	1:A:438:HIS:CD2	2.41	0.56
1:B:1028:ILE:HD13	1:B:1092:ALA:HB1	1.87	0.56
1:D:1847:ILE:HG12	1:D:1870:VAL:HB	1.87	0.56
1:E:3158:LEU:HD11	1:E:3208:VAL:HG21	1.87	0.56
1:A:336:LYS:HB3	1:A:337:PRO:HD2	1.88	0.56
1:B:739:LEU:HD12	1:B:754:ASN:C	2.26	0.56
1:C:1343:LEU:HD23	1:C:1361:LYS:HA	1.88	0.56
1:D:1850:ILE:HB	1:D:1873:MET:CE	2.35	0.56
1:D:2278:GLN:HB2	1:D:2284:ASP:HB2	1.88	0.56
1:H:5028:LEU:HD22	1:H:5057:LEU:HD21	1.87	0.56
1:A:161:LYS:C	1:A:162:ASN:CA	2.68	0.56
1:A:141:ILE:HD11	1:A:194:THR:HG21	1.88	0.56
1:A:269:LYS:HE2	1:A:271:GLU:OE2	2.05	0.56
1:C:1685:VAL:O	1:C:1689:VAL:HG23	2.06	0.56
1:D:1910:ALA:CB	1:D:2038:MET:HG3	2.36	0.56
1:E:3074:ASN:HA	1:E:3112:ASP:HB3	1.88	0.56
1:F:3802:LEU:HD12	1:F:3803:GLY:N	2.21	0.56
1:F:3810:LEU:HB3	1:F:3813:ALA:HB3	1.87	0.56
1:G:4379:LEU:HD12	1:G:4379:LEU:O	2.06	0.56
1:G:4646:ARG:HB3	6:G:6223:HOH:O	2.06	0.56
1:A:295:ASP:O	1:A:298:ILE:HG22	2.06	0.56
1:B:928:GLN:NE2	1:D:2141:ARG:HH11	2.04	0.56
1:F:3756:LEU:HD12	1:F:3757:TRP:N	2.21	0.56
1:F:3829:LYS:HE2	1:F:3856:ILE:HG23	1.87	0.56
1:F:3961:SER:HB2	6:F:6395:HOH:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:4093:MET:CE	1:F:4129:VAL:HG22	2.36	0.56
1:H:4873:MET:HG3	1:H:4887:ILE:HD11	1.87	0.56
1:H:4860:LEU:HD13	1:H:4890:VAL:HA	1.88	0.56
1:B:890:MET:CE	1:B:892:ALA:HB2	2.36	0.55
1:C:1572:GLU:OE1	1:C:1572:GLU:N	2.40	0.55
1:D:1848:CYS:SG	1:D:1868:MET:HB2	2.46	0.55
1:D:2038:MET:CE	1:D:2264:LEU:HD11	2.37	0.55
1:G:4379:LEU:HG	1:G:4380:ILE:HG12	1.88	0.55
1:G:4715:ARG:CB	1:G:4716:PRO:HD2	2.36	0.55
1:H:5118:ARG:HD2	6:H:6689:HOH:O	2.04	0.55
1:H:5281:TRP:CD1	1:H:5316:PRO:HD3	2.41	0.55
1:A:238:MET:CE	1:A:464:LEU:HD22	2.36	0.55
1:A:408:MET:SD	1:A:520:PHE:HD2	2.29	0.55
1:A:510:VAL:HG12	1:A:512:THR:HG23	1.87	0.55
1:B:934:ILE:HG22	1:B:935:LYS:HD3	1.88	0.55
1:E:3506:ASP:O	1:E:3528:PRO:HA	2.06	0.55
1:G:4386:GLN:HB2	1:G:4393:VAL:HB	1.87	0.55
1:C:1374:TYR:O	1:C:1408:VAL:HA	2.05	0.55
1:D:2109:GLN:O	1:D:2113:ILE:HG13	2.05	0.55
1:B:928:GLN:NE2	1:D:2141:ARG:HG2	2.22	0.55
1:D:2176:MET:HE2	1:D:2180:ILE:HG13	1.88	0.55
1:G:4388:GLY:HA3	1:G:4391:PHE:CZ	2.40	0.55
1:H:5092:ALA:HB1	3:H:5333:OXL:C2	2.37	0.55
1:A:141:ILE:CD1	1:A:194:THR:HG21	2.37	0.55
1:A:328:GLN:NE2	1:C:1540:THR:HB	2.22	0.55
1:C:1484:GLU:HG3	6:C:6549:HOH:O	2.06	0.55
1:A:525:ARG:HB2	1:A:525:ARG:HH11	1.71	0.55
1:C:1322:LEU:HD12	1:C:1349:GLU:CG	2.31	0.55
1:G:4222:ALA:CB	1:G:4227:GLU:HG2	2.37	0.55
1:G:4729:VAL:CG1	1:G:4730:PRO:HD2	2.36	0.55
1:A:60:LEU:O	1:A:63:MET:N	2.39	0.55
1:C:1262:GLU:OE2	1:C:1265:LYS:HE3	2.06	0.55
1:E:3191:PHE:CE2	1:E:3193:VAL:HG23	2.36	0.55
1:E:3324:ILE:HG12	1:E:3357:CYS:HB2	1.89	0.55
1:H:4974:TYR:CE2	1:H:5011:PRO:HG3	2.42	0.55
1:H:5314:TRP:HD1	1:H:5315:ARG:HG3	1.69	0.55
1:A:181:SER:O	1:A:182:LEU:HD23	2.06	0.55
1:A:511:LEU:HB3	1:A:521:THR:CG2	2.36	0.55
1:C:1661:GLN:O	1:C:1664:LEU:HB2	2.06	0.55
1:D:2252:VAL:HG21	1:D:2292:ALA:HB2	1.87	0.55
1:F:3941:ARG:NH2	1:H:5094:GLY:O	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:5245:PRO:HG2	1:H:5249:ILE:HD11	1.88	0.55
1:B:706:PRO:O	1:B:1063:HIS:HE1	1.88	0.55
1:B:1080:ALA:HB3	1:B:1083:GLU:CD	2.27	0.55
1:B:999:ARG:NH1	1:D:1823:ASP:HB2	2.21	0.55
1:C:1280:HIS:NE2	1:C:1427:ASP:OD1	2.36	0.55
1:D:2045:ARG:HG2	1:D:2072:ASN:HD21	1.72	0.55
1:D:1902:ILE:CG1	1:D:2295:VAL:HG22	2.34	0.55
1:G:4571:LEU:O	1:G:4575:ARG:HG3	2.07	0.55
1:C:1431:GLY:O	1:C:1436:VAL:HG22	2.07	0.55
1:E:3160:TYR:HB3	1:E:3163:ILE:HG22	1.89	0.55
1:G:4729:VAL:HG13	1:G:4730:PRO:HD2	1.88	0.55
1:B:1067:GLY:HA3	6:B:7611:HOH:O	2.06	0.54
1:B:617:LEU:O	1:B:621:MET:HG2	2.07	0.54
1:C:1532:SER:OG	1:C:1540:THR:HG23	2.07	0.54
1:D:1945:ASN:HD21	1:D:1961:LYS:HZ1	1.55	0.54
1:D:2281:TRP:CH2	1:D:2316:PRO:HA	2.42	0.54
1:E:3495:VAL:O	1:E:3498:ALA:HB3	2.07	0.54
1:H:4847:ILE:HG21	1:H:5159:MET:CE	2.37	0.54
1:D:1985:LYS:HB2	1:D:1993:VAL:O	2.07	0.54
1:E:3192:LEU:N	1:E:3192:LEU:HD22	2.22	0.54
1:E:3525:ARG:HD3	1:F:4114:TRP:CE3	2.42	0.54
1:H:4877:HIS:O	1:H:4883:HIS:NE2	2.37	0.54
1:H:4920:THR:O	1:H:5005:LYS:HA	2.06	0.54
1:H:5239:GLN:OE1	1:H:5242:ARG:HD3	2.06	0.54
1:A:296:LEU:O	1:A:300:ILE:HG12	2.06	0.54
1:A:393:LEU:HG	1:A:397:LEU:HD22	1.88	0.54
1:E:3167:VAL:HG22	1:E:3171:SER:CB	2.37	0.54
1:G:4564:THR:HA	1:G:4570:PRO:HB3	1.89	0.54
1:F:3904:LYS:HD3	1:H:5183:GLU:CD	2.28	0.54
1:A:51:GLY:C	1:A:55:ARG:HG3	2.26	0.54
1:B:673:MET:HE3	1:B:686:THR:HG22	1.88	0.54
1:E:3160:TYR:HB3	1:E:3163:ILE:CG2	2.37	0.54
1:F:4055:ASN:HB3	1:F:4058:THR:HB	1.89	0.54
1:F:4096:GLY:HA3	1:F:4102:PHE:CZ	2.42	0.54
1:G:4691:LEU:O	1:G:4695:VAL:HG23	2.08	0.54
1:A:144:ASP:HB3	1:A:147:TYR:CD1	2.43	0.54
1:A:451:ALA:HB2	1:A:468:ILE:CG2	2.37	0.54
1:B:1103:LYS:HG3	1:B:1106:ASP:OD2	2.07	0.54
1:C:1477:ARG:NH2	1:C:1478:ARG:NH1	2.47	0.54
1:D:2046:LYS:NZ	1:D:2049:ASP:OD1	2.35	0.54
1:D:2135:LYS:O	1:D:2169:TYR:HE2	1.91	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2275:ASP:HB2	1:D:2287:LEU:HD21	1.89	0.54
1:G:4217:LEU:O	1:G:4221:MET:HG2	2.07	0.54
1:A:163:ILE:HA	1:A:166:VAL:HB	1.89	0.54
1:A:294:GLY:CA	1:A:327:THR:HG21	2.37	0.54
1:A:79:THR:OG1	1:A:81:GLU:N	2.40	0.54
1:B:1031:THR:CG2	1:B:1034:GLY:HA2	2.38	0.54
1:C:1434:GLN:OE1	1:C:1434:GLN:HA	2.08	0.54
1:F:3638:PRO:HG3	1:F:3983:GLU:CD	2.28	0.54
1:F:3755:ILE:HG12	1:F:3755:ILE:O	2.07	0.54
1:G:4363:ILE:HG23	1:G:4364:CYS:N	2.23	0.54
1:G:4628:ILE:HD13	1:G:4692:ALA:CB	2.37	0.54
1:A:181:SER:C	1:A:182:LEU:HD23	2.28	0.54
1:A:489:VAL:O	1:A:493:MET:HG2	2.07	0.54
1:B:686:THR:O	1:B:690:VAL:HG23	2.08	0.54
1:B:788:GLY:HA3	1:B:791:PHE:CE1	2.42	0.54
1:C:1255:ARG:HH22	1:C:1285:GLU:HB3	1.71	0.54
1:E:3221:SER:O	1:E:3224:ASP:HB2	2.07	0.54
1:E:3259:GLU:O	1:E:3262:LYS:HG2	2.08	0.54
1:F:3845:ARG:CG	1:F:3874:GLU:HB3	2.38	0.54
1:C:1681:TRP:CH2	1:C:1716:PRO:HA	2.43	0.54
1:D:2252:VAL:CG2	1:D:2292:ALA:HB2	2.38	0.54
1:G:4483:LEU:O	1:G:4521:LYS:NZ	2.40	0.54
1:G:4652:VAL:HG21	1:G:4692:ALA:HB2	1.89	0.54
1:H:4887:ILE:N	1:H:4887:ILE:HD13	2.22	0.54
1:A:511:LEU:HD22	1:A:521:THR:CG2	2.37	0.54
1:A:514:TRP:N	1:A:522:ASN:HD21	1.93	0.54
1:D:1902:ILE:C	1:D:1903:LEU:HD23	2.28	0.54
1:D:1980:ILE:HD11	1:D:2000:GLY:HA3	1.90	0.54
1:F:3910:LYS:NZ	1:H:5149:ASN:HD21	2.06	0.54
1:E:3407:LEU:HG	1:F:4126:VAL:HG11	1.90	0.54
1:A:432:GLU:O	1:A:458:THR:HG21	2.08	0.54
1:B:654:SER:HA	1:B:659:THR:HG21	1.90	0.54
1:C:1213:GLN:HA	1:C:1213:GLN:OE1	2.08	0.54
1:C:1326:SER:HB3	1:C:1329:ALA:HB3	1.90	0.54
1:C:1347:TYR:HE2	1:C:1355:ILE:CD1	2.21	0.54
1:C:1561:SER:HB2	6:C:6410:HOH:O	2.07	0.54
1:D:1940:LYS:HE3	1:D:1991:PHE:CG	2.43	0.54
1:D:2296:GLY:HA3	1:D:2302:PHE:CZ	2.43	0.54
1:E:3080:HIS:HE1	1:E:3227:ASP:OD1	1.91	0.54
1:G:4212:ILE:HD13	1:G:4233:ASP:OD2	2.08	0.54
1:G:4437:ASP:OD1	1:G:4660:ARG:HD2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1833:ASP:HA	6:D:6995:HOH:O	2.07	0.53
1:E:3068:MET:HE1	1:E:3071:ALA:CB	2.36	0.53
1:G:4257:VAL:HG23	1:G:4289:ASN:HB3	1.90	0.53
1:A:224:ASP:O	1:A:228:LEU:HG	2.08	0.53
1:C:1421:SER:O	1:C:1424:ASP:HB2	2.09	0.53
1:D:1958:LEU:CD1	1:D:1963:ILE:HD13	2.38	0.53
1:D:2008:VAL:HG12	1:D:2010:LEU:CD2	2.38	0.53
1:G:4451:HIS:O	1:G:4455:LYS:HG2	2.08	0.53
1:A:87:ILE:HG22	1:A:91:ARG:HD2	1.91	0.53
1:B:618:HIS:CE1	1:B:631:ARG:HD3	2.43	0.53
1:C:1348:MET:HA	1:C:1357:TRP:CG	2.44	0.53
1:C:1518:ARG:HD2	6:C:6442:HOH:O	2.07	0.53
1:C:1571:LEU:O	1:C:1575:ARG:HG3	2.08	0.53
1:F:3867:ILE:HD13	1:F:3867:ILE:N	2.24	0.53
1:F:3939:PRO:HG3	1:F:3976:MET:HG2	1.90	0.53
1:G:4270:VAL:HG22	1:G:4308:ALA:HB3	1.90	0.53
1:B:716:PRO:HG2	1:B:843:PHE:CB	2.38	0.53
1:C:1611:MET:SD	1:D:2326:VAL:HG23	2.49	0.53
1:D:2176:MET:HA	1:D:2176:MET:CE	2.31	0.53
1:D:1839:ILE:O	1:D:2182:ARG:HD2	2.09	0.53
1:D:2288:ARG:O	1:D:2291:LEU:HB3	2.08	0.53
1:E:3306:PHE:HA	6:E:7081:HOH:O	2.08	0.53
1:C:1362:ASN:ND2	1:C:1365:LYS:HB2	2.24	0.53
1:C:1516:CYS:HB3	1:C:1521:LYS:O	2.09	0.53
1:H:5130:LEU:HD23	1:H:5143:GLU:HB3	1.88	0.53
1:A:172:LYS:HE3	1:A:197:GLU:OE1	2.09	0.53
1:C:1250:ILE:HD13	1:C:1250:ILE:N	2.24	0.53
1:C:1248:CYS:CB	1:C:1268:MET:HE3	2.26	0.53
1:F:3642:ARG:HB2	1:F:3982:ARG:HG3	1.91	0.53
1:G:4661:GLN:O	1:G:4664:LEU:HB2	2.09	0.53
1:H:4923:ILE:O	1:H:4925:GLY:N	2.42	0.53
1:H:5130:LEU:CD1	1:H:5133:MET:HE1	2.25	0.53
1:C:1650:ILE:HD12	1:C:1669:PHE:HB2	1.90	0.53
1:F:3732:GLU:HB2	1:F:3801:PHE:CE1	2.44	0.53
1:G:4250:ILE:HD11	1:G:4268:MET:HE3	1.89	0.53
1:G:4531:GLU:O	1:G:4534:ILE:HD12	2.09	0.53
1:A:188:GLY:HA3	1:A:191:PHE:CD1	2.43	0.53
1:C:1293:ALA:O	1:C:1296:SER:OG	2.26	0.53
1:F:3663:MET:HE2	1:F:3668:MET:HE1	1.91	0.53
1:G:4336:GLY:HA2	1:G:4395:GLU:CD	2.29	0.53
1:H:5023:LYS:NZ	1:H:5027:ASP:OD2	2.30	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:GLY:O	1:C:1538:ARG:NH1	2.42	0.53
1:B:804:SER:O	1:B:806:LYS:HD3	2.09	0.53
1:B:928:GLN:HB2	1:D:2141:ARG:HB2	1.91	0.53
1:D:2064:ILE:HD11	6:D:7350:HOH:O	2.09	0.53
1:D:2281:TRP:CD1	1:D:2316:PRO:HD3	2.44	0.53
1:F:3683:HIS:O	1:F:3687:ILE:HG13	2.09	0.53
1:A:102:ILE:HG22	1:A:103:LEU:CD1	2.39	0.53
1:A:27:GLU:O	1:A:31:ARG:HG3	2.08	0.53
1:A:454:ARG:CG	1:A:473:CYS:HB3	2.39	0.53
1:A:487:LEU:C	1:A:487:LEU:HD23	2.29	0.53
1:C:1532:SER:O	1:C:1534:ILE:N	2.40	0.53
1:C:1555:ALA:O	1:C:1666:ARG:NH1	2.35	0.53
1:D:1987:LYS:HA	1:D:1992:LEU:HD23	1.90	0.53
1:F:3650:ILE:CG1	1:F:3673:MET:HE1	2.39	0.53
1:F:4066:ARG:HG3	1:F:4067:GLY:N	2.22	0.53
1:H:5073:HIS:CE1	1:H:5100:ILE:HG22	2.44	0.53
1:B:815:VAL:HG21	1:B:843:PHE:HE2	1.73	0.52
1:C:1379:LEU:HG	1:C:1380:ILE:HG12	1.90	0.52
1:G:4445:ARG:N	1:G:4449:ASP:OD2	2.29	0.52
1:A:425:ALA:HB1	1:A:502:PHE:HB3	1.92	0.52
1:B:720:THR:HG22	1:B:758:LEU:HD21	1.90	0.52
1:C:1255:ARG:NH2	1:C:1285:GLU:HB3	2.23	0.52
1:C:1675:ASP:CB	1:C:1676:PRO:HD2	2.38	0.52
1:F:3653:ALA:CB	1:F:3966:LYS:HA	2.39	0.52
1:G:4276:SER:HB3	1:G:4319:ARG:NE	2.20	0.52
1:G:4452:GLU:O	1:G:4456:ILE:HG12	2.09	0.52
1:B:815:VAL:HG22	6:B:6888:HOH:O	2.08	0.52
1:G:4260:LEU:HD23	1:G:4263:MET:HG3	1.91	0.52
1:H:4945:ASN:HB3	1:H:4948:MET:CE	2.40	0.52
1:A:87:ILE:O	1:A:91:ARG:HG3	2.10	0.52
1:C:1323:ILE:HG21	1:C:1331:VAL:HG23	1.91	0.52
1:C:1428:LEU:HD12	1:C:1456:ILE:HG21	1.90	0.52
1:E:3113:THR:HG22	1:E:3242:SER:H	1.74	0.52
1:E:3133:LEU:HD22	1:E:3202:LEU:HB2	1.92	0.52
1:G:4274:ASN:OD1	1:G:4276:SER:HB2	2.10	0.52
1:C:1372:LYS:HA	1:C:1382:LEU:O	2.10	0.52
1:C:1472:ASN:HD22	1:C:1475:GLY:H	1.57	0.52
1:D:1860:LEU:HB3	1:D:1893:ALA:CB	2.39	0.52
1:H:4843:ASN:HB3	1:H:5267:GLY:CA	2.39	0.52
1:A:334:ILE:HG23	1:A:367:GLY:HA2	1.92	0.52
1:E:3017:LEU:O	1:E:3020:ALA:HB3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3493:MET:HE3	1:E:3529:VAL:HG13	1.91	0.52
1:F:4075:ASP:HB2	1:F:4087:LEU:HD21	1.91	0.52
1:G:4608:MET:SD	1:G:4721:THR:HG22	2.49	0.52
1:B:1054:ARG:HG2	1:B:1073:CYS:HB3	1.91	0.52
1:F:4104:LYS:HG3	1:F:4130:PRO:C	2.30	0.52
1:G:4221:MET:HE3	1:G:4221:MET:HA	1.91	0.52
1:A:454:ARG:NH2	1:A:484:ASP:OD2	2.42	0.52
1:B:847:ALA:N	1:B:881:GLU:OE1	2.30	0.52
1:C:1326:SER:CB	1:C:1329:ALA:HB2	2.40	0.52
1:C:1431:GLY:HA2	1:C:1434:GLN:HB2	1.92	0.52
1:C:1621:LYS:NZ	1:D:2201:SER:O	2.43	0.52
1:D:2230:LEU:HD22	1:D:2312:THR:HG22	1.91	0.52
1:H:4932:GLU:OE1	1:H:4934:LYS:HG2	2.10	0.52
1:A:210:LEU:HB3	1:A:213:ALA:HB2	1.92	0.52
1:A:292:ALA:HB1	3:A:533:OXL:C2	2.39	0.52
1:A:480:ALA:HB3	1:A:483:GLU:HB2	1.90	0.52
1:B:731:VAL:CG1	1:B:753:GLU:HB3	2.40	0.52
1:D:2280:ALA:HB3	1:D:2283:GLU:HG3	1.90	0.52
1:E:3496:GLY:O	1:E:3501:PHE:N	2.37	0.52
1:G:4410:LEU:HD12	1:G:4410:LEU:N	2.24	0.52
1:H:4851:GLY:HA3	1:H:5165:ALA:O	2.10	0.52
1:A:123:ILE:O	1:A:129:ALA:HB3	2.10	0.52
1:A:308:ALA:O	1:A:312:ILE:HG13	2.10	0.52
1:C:1252:PRO:HD2	1:C:1565:ALA:O	2.09	0.52
1:E:3145:ASN:N	1:E:3145:ASN:HD22	2.08	0.52
1:G:4333:LEU:N	1:G:4333:LEU:HD23	2.25	0.52
1:G:4522:PRO:HG3	1:G:4665:TYR:CE2	2.44	0.52
1:H:5133:MET:HE2	1:H:5139:PRO:HB3	1.92	0.52
1:A:176:ASP:HB3	1:A:179:LEU:HB3	1.92	0.51
1:A:300:ILE:HB	1:A:301:PRO:HD2	1.91	0.51
1:D:2046:LYS:HB3	1:D:2081:GLU:OE2	2.10	0.51
1:D:2094:GLY:CA	1:D:2127:THR:HG21	2.39	0.51
1:F:3971:LEU:O	1:F:3975:ARG:HG3	2.10	0.51
1:A:456:HIS:CD2	1:A:456:HIS:N	2.79	0.51
1:A:69:ASN:HB3	1:A:463:HIS:CE1	2.44	0.51
1:C:1687:LEU:HG	1:C:1688:ARG:N	2.24	0.51
1:D:1958:LEU:CD2	1:D:2008:VAL:HG21	2.40	0.51
1:E:3453:THR:CG2	1:E:3459:ALA:HB2	2.40	0.51
1:F:3724:LYS:C	1:F:3726:SER:H	2.14	0.51
1:H:4988:GLY:HA3	1:H:4991:PHE:CE2	2.45	0.51
1:H:5133:MET:HE3	1:H:5139:PRO:HB3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:LEU:HD23	1:A:111:LEU:C	2.30	0.51
1:F:3894:GLY:CA	1:F:3927:THR:HG21	2.41	0.51
1:H:5096:LEU:O	1:H:5100:ILE:HG12	2.11	0.51
1:A:126:SER:CB	1:A:129:ALA:HB2	2.28	0.51
1:A:293:ARG:HD3	1:A:326:ALA:O	2.11	0.51
1:A:392:LYS:O	1:A:396:GLU:HG3	2.11	0.51
1:A:398:ALA:HA	1:A:413:MET:HE3	1.91	0.51
1:B:756:LEU:HD13	1:B:758:LEU:HD21	1.92	0.51
1:C:1367:VAL:O	1:C:1387:LYS:NZ	2.36	0.51
1:C:1531:GLU:OE1	1:C:1531:GLU:HA	2.10	0.51
1:A:252:GLU:O	1:A:255:LYS:N	2.42	0.51
1:A:333:MET:HE2	1:A:373:ALA:HA	1.91	0.51
1:B:656:SER:O	1:B:660:LEU:HB2	2.10	0.51
1:D:1954:ASN:O	1:D:1955:ILE:HG13	2.09	0.51
1:D:2083:LEU:HD21	1:D:2119:ALA:CB	2.41	0.51
1:D:2141:ARG:HG2	1:D:2141:ARG:NH1	2.21	0.51
1:D:2225:ALA:HB1	1:D:2302:PHE:HB3	1.93	0.51
1:B:931:GLU:HA	1:B:931:GLU:OE1	2.11	0.51
1:D:1854:SER:O	1:D:1860:LEU:HD13	2.09	0.51
1:D:1966:VAL:O	1:D:1966:VAL:HG23	2.10	0.51
1:E:3164:CYS:O	1:E:3187:LYS:CE	2.59	0.51
1:E:3300:ILE:HB	1:E:3301:PRO:HD2	1.92	0.51
1:F:3783:GLN:O	1:F:3794:THR:HA	2.11	0.51
1:A:172:LYS:HE3	1:A:197:GLU:CD	2.30	0.51
1:A:283:LEU:HD22	1:A:283:LEU:O	2.11	0.51
1:A:495:VAL:HG11	1:A:499:ARG:HH11	1.75	0.51
1:C:1227:GLU:O	1:C:1231:ARG:HG3	2.10	0.51
1:C:1429:LYS:HB3	6:C:7020:HOH:O	2.11	0.51
1:D:1902:ILE:O	1:D:1903:LEU:HD23	2.11	0.51
1:D:1952:ASP:OD1	1:D:1954:ASN:N	2.42	0.51
1:D:2191:ARG:HD2	1:D:2191:ARG:C	2.30	0.51
1:F:3699:SER:O	1:F:3701:PRO:HD3	2.11	0.51
1:F:3881:GLU:HG3	1:F:3882:ILE:N	2.25	0.51
1:G:4370:GLY:N	1:G:4384:VAL:O	2.31	0.51
1:H:5015:VAL:HG11	1:H:5017:LEU:HD12	1.92	0.51
1:A:186:GLN:HB2	1:A:193:VAL:HB	1.93	0.51
1:A:53:ALA:HB2	1:A:366:LYS:HA	1.91	0.51
1:B:1091:LEU:C	1:B:1091:LEU:HD12	2.31	0.51
1:B:614:THR:O	1:B:617:LEU:HG	2.11	0.51
1:C:1696:GLY:HA3	1:C:1702:PHE:CZ	2.46	0.51
1:F:4075:ASP:HB3	1:F:4076:PRO:CD	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:ASN:HB2	1:A:162:ASN:N	2.24	0.51
1:A:173:VAL:N	1:A:182:LEU:O	2.30	0.51
1:C:1243:ASN:H	1:C:1585:GLU:CD	2.13	0.51
1:C:1247:ILE:HB	1:C:1559:MET:HG3	1.92	0.51
1:F:3739:LEU:HD21	1:F:3756:LEU:CB	2.41	0.51
1:F:3821:SER:O	1:F:3824:ASP:HB2	2.11	0.51
1:F:4104:LYS:HA	1:F:4129:VAL:O	2.11	0.51
1:H:4850:ILE:HD11	1:H:4868:MET:HE3	1.90	0.51
1:H:4974:TYR:HB2	1:H:5009:ASN:HB2	1.92	0.51
1:A:210:LEU:HB2	1:A:213:ALA:HB3	1.93	0.51
1:A:238:MET:HE2	1:A:464:LEU:CD2	2.41	0.51
1:A:411:MET:HG2	1:A:521:THR:O	2.11	0.51
1:C:1302:ILE:HA	1:C:1695:VAL:HG22	1.93	0.51
1:D:2042:SER:HA	1:D:2069:LYS:HE2	1.91	0.51
1:D:2304:LYS:HG3	1:D:2330:PRO:O	2.09	0.51
1:E:3068:MET:CE	1:E:3071:ALA:HB2	2.40	0.51
1:G:4636:SER:O	1:G:4639:GLN:HB2	2.11	0.51
1:H:5115:ARG:NH2	6:H:6799:HOH:O	2.44	0.51
1:A:122:LEU:CD2	1:A:204:SER:HB3	2.21	0.50
1:A:34:ILE:HD13	1:C:1476:VAL:HG11	1.93	0.50
1:B:1087:LEU:C	1:B:1087:LEU:HD23	2.31	0.50
1:C:1360:TYR:CE2	1:C:1366:VAL:HG11	2.44	0.50
1:D:2240:VAL:HG12	1:D:2249:ILE:HD11	1.92	0.50
1:E:3160:TYR:CD2	1:E:3163:ILE:N	2.79	0.50
1:F:3893:ARG:HH22	1:F:3946:ASP:CG	2.14	0.50
1:G:4387:LYS:HG3	1:G:4392:LEU:HD11	1.93	0.50
1:G:4444:ILE:HD12	1:G:4449:ASP:HB2	1.93	0.50
1:G:4493:ARG:NH1	1:G:4529:MET:HG2	2.26	0.50
1:G:4241:ALA:HB2	1:G:4701:PHE:CE1	2.46	0.50
1:A:330:LEU:HD22	1:A:377:GLN:HG3	1.92	0.50
1:C:1343:LEU:HD23	1:C:1361:LYS:HD3	1.93	0.50
1:C:1612:ALA:O	1:C:1616:VAL:HG23	2.11	0.50
1:C:1665:TYR:N	1:C:1665:TYR:CD1	2.80	0.50
1:F:3762:ASN:OD1	1:F:3765:LYS:HD3	2.11	0.50
1:A:330:LEU:CD2	1:A:377:GLN:HG3	2.42	0.50
1:E:3274:GLU:O	1:E:3278:ARG:HG3	2.12	0.50
1:G:4322:LEU:C	1:G:4351:CYS:HB2	2.31	0.50
1:G:4351:CYS:O	1:G:4352:ASP:HB3	2.11	0.50
1:A:57:VAL:HG22	1:A:89:ASN:CB	2.42	0.50
1:C:1715:ARG:HB3	1:C:1716:PRO:CD	2.40	0.50
1:E:3022:ALA:HB1	1:E:3027:GLU:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3198:ASN:HD21	1:G:4538:ARG:HH22	1.58	0.50
1:F:3688:LYS:HG2	6:F:7588:HOH:O	2.11	0.50
1:F:3711:LEU:HD23	1:F:3711:LEU:C	2.31	0.50
1:F:3893:ARG:HA	1:F:3896:LEU:HB3	1.92	0.50
1:H:4868:MET:HE1	1:H:4871:ALA:HA	1.93	0.50
1:A:520:PHE:N	1:A:520:PHE:CD1	2.79	0.50
1:G:4345:ASN:O	1:G:4348:MET:HG3	2.10	0.50
1:G:4474:GLU:O	1:G:4478:ARG:HG3	2.11	0.50
1:H:4945:ASN:O	1:H:4948:MET:HB2	2.11	0.50
1:C:1272:ARG:NE	1:C:1312:ASP:OD2	2.41	0.50
1:C:1671:VAL:CG1	1:C:1691:LEU:HD21	2.39	0.50
1:F:3634:ILE:HG23	6:F:6928:HOH:O	2.11	0.50
1:F:3673:MET:HE2	1:F:3673:MET:HA	1.94	0.50
1:C:1654:ARG:HG2	1:C:1673:CYS:O	2.12	0.50
1:D:1861:LYS:O	1:D:1865:LYS:HG3	2.12	0.50
1:D:2190:HIS:HD2	6:D:6448:HOH:O	1.94	0.50
1:G:4504:LYS:O	1:G:4507:LEU:HB2	2.12	0.50
1:G:4621:LYS:HD2	1:G:4621:LYS:O	2.12	0.50
1:G:4243:ASN:CB	1:G:4667:GLY:HA2	2.41	0.50
1:A:343:GLU:O	1:A:347:VAL:HG23	2.11	0.50
1:A:456:HIS:CD2	1:A:456:HIS:H	2.27	0.50
1:A:57:VAL:HG11	1:A:92:THR:HG22	1.94	0.50
1:B:720:THR:HG22	1:B:758:LEU:HD23	1.89	0.50
1:C:1345:ASN:C	1:C:1347:TYR:H	2.15	0.50
1:D:2057:LEU:HB2	6:D:7479:HOH:O	2.11	0.50
1:E:3135:LYS:HA	1:E:3196:VAL:HG12	1.93	0.50
1:G:4276:SER:CB	1:G:4319:ARG:HH21	2.24	0.50
1:G:4647:ALA:HB1	1:G:4648:PRO:HD2	1.92	0.50
1:D:2192:LYS:HB2	6:D:7514:HOH:O	2.12	0.50
1:D:2206:ASP:HB3	1:D:2209:GLU:OE1	2.12	0.50
1:E:3456:HIS:N	1:E:3456:HIS:CD2	2.79	0.50
1:A:123:ILE:HD11	1:A:202:LEU:CD2	2.42	0.49
1:A:511:LEU:HB3	1:A:521:THR:HG21	1.93	0.49
1:B:1056:HIS:H	1:B:1056:HIS:CD2	2.30	0.49
1:C:1247:ILE:HG23	1:C:1270:VAL:HB	1.94	0.49
1:C:1363:ILE:HA	1:C:1366:VAL:CG1	2.42	0.49
1:D:2113:ILE:HD13	1:D:2155:ALA:HB2	1.93	0.49
1:G:4391:PHE:CE1	1:G:4393:VAL:HG23	2.47	0.49
1:A:191:PHE:O	1:A:192:LEU:HD13	2.11	0.49
1:A:391:ARG:HD3	6:A:6393:HOH:O	2.10	0.49
1:A:409:GLU:O	1:A:413:MET:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:ALA:HB2	1:A:468:ILE:HG23	1.94	0.49
1:A:469:PHE:CD1	1:A:469:PHE:N	2.81	0.49
1:C:1421:SER:N	1:C:1424:ASP:HB2	2.27	0.49
1:D:1916:PRO:HG3	1:D:2045:ARG:NH2	2.27	0.49
1:F:3899:GLU:HB3	6:F:7535:HOH:O	2.11	0.49
1:F:4104:LYS:HB2	1:F:4130:PRO:O	2.12	0.49
1:G:4522:PRO:HG3	1:G:4665:TYR:CZ	2.48	0.49
1:G:4243:ASN:HB3	1:G:4667:GLY:HA2	1.92	0.49
1:A:75:PHE:CE1	1:A:111:LEU:HG	2.47	0.49
1:A:145:ASN:C	1:A:147:TYR:H	2.15	0.49
1:C:1492:ALA:HB1	3:C:1733:OXL:C2	2.42	0.49
1:B:941:ARG:N	1:D:2128:GLN:NE2	2.59	0.49
1:E:3209:ASN:O	1:E:3211:PRO:HD3	2.12	0.49
1:F:3955:ALA:O	1:F:4066:ARG:NH1	2.38	0.49
1:F:4122:ASN:N	1:F:4122:ASN:OD1	2.45	0.49
1:G:4322:LEU:HD22	1:G:4326:SER:O	2.12	0.49
1:G:4625:ALA:HB1	1:G:4702:PHE:HB3	1.94	0.49
1:C:1428:LEU:CD1	1:C:1456:ILE:HB	2.40	0.49
1:G:4222:ALA:HB1	1:G:4227:GLU:HB3	1.95	0.49
1:G:4611:MET:CE	1:G:4724:MET:HB2	2.41	0.49
1:G:4725:ARG:HD3	1:H:5314:TRP:CE3	2.47	0.49
1:A:453:THR:CG2	1:A:459:ALA:HB2	2.42	0.49
1:C:1287:ILE:O	1:C:1290:VAL:HB	2.11	0.49
1:C:1342:THR:O	1:C:1357:TRP:HA	2.11	0.49
1:C:1479:PHE:CE1	1:C:1489:ILE:HD12	2.45	0.49
1:D:1958:LEU:HD12	1:D:1963:ILE:HD13	1.94	0.49
1:E:3073:MET:CE	1:E:3109:VAL:HG13	2.42	0.49
1:E:3167:VAL:HG22	1:E:3171:SER:HB2	1.95	0.49
1:H:4847:ILE:CB	1:H:5159:MET:HE3	2.42	0.49
1:A:240:PHE:HB3	1:A:269:LYS:HD2	1.94	0.49
1:B:1078:GLN:HA	1:B:1078:GLN:HE21	1.78	0.49
1:B:928:GLN:HE22	1:D:2141:ARG:HH11	1.58	0.49
1:C:1656:HIS:HB3	1:C:1660:ARG:HH21	1.78	0.49
1:D:1940:LYS:HE3	1:D:1991:PHE:CB	2.43	0.49
1:D:2110:LYS:NZ	6:D:6361:HOH:O	2.44	0.49
1:E:3322:PRO:HG3	1:E:3465:TYR:CE2	2.47	0.49
1:F:3717:GLU:HG3	1:F:3843:PHE:HE2	1.78	0.49
1:G:4333:LEU:C	1:G:4334:LYS:HG2	2.33	0.49
1:G:4372:LYS:HE2	1:G:4397:GLU:OE1	2.13	0.49
1:H:4979:LEU:HD12	1:H:4979:LEU:O	2.13	0.49
1:A:64:ILE:CD1	1:A:94:THR:HA	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:SER:HB2	1:B:1021:LYS:HZ3	1.77	0.49
1:B:781:SER:HB3	1:B:798:ASN:HB2	1.94	0.49
1:C:1335:LYS:HG3	1:C:1336:GLY:N	2.28	0.49
1:G:4377:ASP:HA	1:G:4498:ILE:HD11	1.95	0.49
1:G:4443:PHE:O	1:G:4445:ARG:HG3	2.12	0.49
1:G:4570:PRO:O	1:G:4574:VAL:HG23	2.12	0.49
1:B:911:MET:HE2	6:D:7520:HOH:O	2.13	0.49
1:G:4506:PHE:HB2	6:G:7537:HOH:O	2.13	0.49
1:G:4645:PRO:HD2	6:G:7272:HOH:O	2.13	0.49
1:H:5296:GLY:HA3	1:H:5302:PHE:CZ	2.48	0.49
1:A:215:VAL:CG2	1:A:217:LEU:HD12	2.43	0.49
1:A:235:ASP:OD1	1:A:235:ASP:O	2.30	0.49
1:B:1009:GLU:O	1:B:1013:MET:HG3	2.13	0.49
1:D:1877:HIS:CE1	5:D:2335:ATP:H2'	2.48	0.49
1:G:4714:TRP:HA	1:G:4714:TRP:CE3	2.48	0.49
1:H:4942:THR:CG2	1:H:4944:ASP:H	2.11	0.49
1:C:1347:TYR:HE2	1:C:1355:ILE:HD12	1.78	0.49
1:C:1357:TRP:CE3	1:C:1358:LEU:N	2.81	0.49
1:C:1479:PHE:CZ	1:C:1483:LEU:HG	2.48	0.49
1:C:1601:SER:OG	1:D:2221:LYS:NZ	2.46	0.49
1:D:2203:HIS:N	1:D:2203:HIS:ND1	2.61	0.49
1:E:3391:ARG:O	1:E:3395:GLU:HG3	2.13	0.49
1:H:4845:GLY:N	6:H:6157:HOH:O	2.45	0.49
1:A:93:ALA:O	1:A:96:SER:HB3	2.13	0.48
1:C:1294:THR:HG22	1:C:1295:GLU:OE1	2.12	0.48
1:C:1706:ASP:O	1:C:1728:PRO:HA	2.12	0.48
1:D:1937:ALA:O	1:D:1996:VAL:HG23	2.13	0.48
1:E:3242:SER:HA	1:E:3269:LYS:HE2	1.95	0.48
1:G:4503:GLU:N	1:G:4503:GLU:OE1	2.41	0.48
1:H:4821:MET:HE3	1:H:4821:MET:HA	1.94	0.48
1:H:4873:MET:CE	1:H:4887:ILE:HD12	2.43	0.48
1:A:47:ILE:HB	1:A:359:MET:HG3	1.94	0.48
1:C:1602:SER:HB2	1:D:1821:MET:CE	2.43	0.48
1:C:1628:ILE:HD13	1:C:1692:ALA:HB3	1.95	0.48
1:B:624:THR:HB	1:D:2196:GLU:CD	2.33	0.48
1:E:3283:LEU:HD22	1:E:3283:LEU:O	2.12	0.48
1:F:3662:GLU:O	1:F:3666:SER:OG	2.29	0.48
1:G:4334:LYS:O	1:G:4337:ALA:HB3	2.13	0.48
1:A:77:HIS:CE1	5:A:535:ATP:H3'	2.49	0.48
1:A:57:VAL:HG23	1:A:89:ASN:CG	2.33	0.48
1:B:976:MET:HE3	1:B:980:ILE:HG13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1609:GLU:HB3	1:D:2221:LYS:HE2	1.95	0.48
1:E:3163:ILE:O	1:E:3163:ILE:HG23	2.13	0.48
1:F:3694:THR:HG22	1:F:3704:TYR:OH	2.12	0.48
1:F:3817:LEU:HD22	1:F:3818:PRO:HD2	1.95	0.48
1:F:3933:MET:HA	1:F:3936:LYS:O	2.13	0.48
1:E:3028:HIS:HE1	6:E:6278:HOH:O	1.96	0.48
1:E:3273:HIS:CE1	1:E:3300:ILE:HG22	2.49	0.48
1:F:3623:ASP:N	1:F:3623:ASP:OD1	2.45	0.48
1:F:3663:MET:HE2	1:F:3668:MET:CE	2.43	0.48
1:F:3731:VAL:HG13	1:F:3732:GLU:N	2.29	0.48
1:F:3789:PRO:HD2	1:F:3791:PHE:CE1	2.48	0.48
1:F:3845:ARG:HG2	1:F:3874:GLU:CB	2.43	0.48
1:G:4322:LEU:HB2	1:G:4349:GLU:HA	1.94	0.48
1:H:5238:HIS:NE2	6:H:7259:HOH:O	2.34	0.48
1:A:209:ASN:C	1:A:210:LEU:HD13	2.33	0.48
1:A:237:ASP:O	1:A:461:GLN:NE2	2.45	0.48
1:B:870:ILE:HG21	1:B:912:ILE:HD11	1.95	0.48
1:B:923:VAL:HG22	1:B:924:ILE:N	2.29	0.48
1:E:3083:HIS:O	1:E:3087:ILE:HG13	2.14	0.48
1:F:3820:VAL:HG21	1:F:3852:GLU:HB3	1.95	0.48
1:H:5015:VAL:HG12	1:H:5017:LEU:H	1.78	0.48
1:A:80:HIS:CE1	1:A:230:PHE:HB2	2.48	0.48
1:E:3068:MET:HE2	1:E:3071:ALA:HA	1.96	0.48
1:E:3142:THR:CG2	1:E:3144:ASP:H	1.99	0.48
1:E:3294:GLY:CA	1:E:3327:THR:HG21	2.44	0.48
1:E:3509:ILE:HD13	1:E:3526:VAL:HG23	1.93	0.48
1:F:3815:VAL:O	1:F:3817:LEU:N	2.46	0.48
1:C:1376:ASP:CG	1:C:1406:LYS:HE2	2.32	0.48
1:F:3817:LEU:HD23	1:F:3817:LEU:HA	1.51	0.48
1:H:4900:ASP:OD2	1:H:4903:LEU:HG	2.14	0.48
1:A:216:ASP:OD1	1:A:216:ASP:O	2.32	0.48
1:A:322:PRO:HG3	1:A:465:TYR:CE2	2.48	0.48
1:A:50:ILE:HD13	1:A:50:ILE:N	2.29	0.48
1:A:77:HIS:CD2	5:A:535:ATP:H2'	2.49	0.48
1:B:700:ASP:O	1:B:703:LEU:N	2.46	0.48
1:C:1630:LEU:HD22	1:C:1712:THR:HG22	1.95	0.48
1:C:1671:VAL:HG12	1:C:1691:LEU:CD2	2.41	0.48
1:D:1817:LEU:HA	1:D:1820:ALA:CB	2.44	0.48
1:C:1602:SER:HB2	1:D:1821:MET:HE1	1.95	0.48
1:E:3146:ALA:O	1:E:3150:LYS:HD2	2.14	0.48
1:E:3179:LEU:HB2	6:E:6658:HOH:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4257:VAL:CG2	1:G:4289:ASN:HB3	2.44	0.48
1:A:47:ILE:HG22	1:A:359:MET:HG3	1.94	0.48
1:A:89:ASN:N	1:A:89:ASN:HD22	2.11	0.48
1:C:1421:SER:HB2	1:C:1424:ASP:H	1.79	0.48
1:C:1727:VAL:HG13	1:C:1728:PRO:HD2	1.96	0.48
1:E:3062:GLU:HA	1:E:3062:GLU:OE1	2.12	0.48
1:E:3024:THR:HB	1:G:4596:GLU:CD	2.34	0.48
1:H:5275:ASP:HB3	1:H:5276:PRO:CD	2.43	0.48
1:C:1294:THR:HG22	1:C:1295:GLU:N	2.29	0.48
1:C:1360:TYR:HD2	1:C:1363:ILE:CB	2.27	0.48
1:C:1611:MET:HG3	1:C:1721:THR:O	2.14	0.48
1:D:1819:ALA:HA	1:D:1831:ARG:HD2	1.95	0.48
1:D:1942:THR:O	1:D:1957:TRP:HA	2.14	0.48
1:E:3019:ALA:HA	1:E:3031:ARG:CD	2.44	0.48
1:E:3181:SER:O	1:E:3197:GLU:HB2	2.14	0.48
1:F:3721:GLY:CA	1:F:3757:TRP:HE3	2.26	0.48
1:A:139:LEU:HD21	1:A:156:LEU:HB2	1.95	0.47
1:A:328:GLN:HE22	1:C:1540:THR:CA	2.26	0.47
1:A:57:VAL:CG1	1:A:92:THR:HG22	2.44	0.47
1:B:873:HIS:ND1	1:B:900:ILE:HG22	2.29	0.47
1:C:1276:SER:HB3	1:C:1319:ARG:NH1	2.28	0.47
1:G:4273:MET:HE3	1:G:4286:THR:CG2	2.43	0.47
1:G:4599:ARG:O	1:G:4602:SER:HB3	2.14	0.47
1:H:5293:MET:O	1:H:5297:LYS:HD3	2.14	0.47
1:A:245:ARG:HG2	1:A:274:GLU:HB3	1.95	0.47
1:B:845:ARG:HD2	6:B:6993:HOH:O	2.14	0.47
1:B:924:ILE:HG12	1:B:957:CYS:HB2	1.95	0.47
1:C:1666:ARG:HG3	1:C:1667:GLY:N	2.28	0.47
1:D:2281:TRP:CZ2	1:D:2316:PRO:HA	2.49	0.47
1:F:3787:LYS:HB3	1:F:3792:LEU:HD11	1.94	0.47
1:G:4275:PHE:HE2	1:G:4280:HIS:CD2	2.32	0.47
1:G:4524:ILE:HG12	1:G:4557:CYS:HB2	1.96	0.47
1:G:4681:TRP:NE1	1:G:4715:ARG:HA	2.28	0.47
1:H:5279:GLU:HG3	1:H:5280:ALA:N	2.30	0.47
1:A:409:GLU:HB3	1:B:1021:LYS:HE2	1.95	0.47
1:C:1360:TYR:CD2	1:C:1363:ILE:HB	2.46	0.47
1:C:1391:PHE:O	1:C:1392:LEU:HD13	2.14	0.47
1:C:1532:SER:C	1:C:1534:ILE:H	2.17	0.47
1:C:1588:MET:SD	1:C:1666:ARG:NH2	2.87	0.47
1:D:2190:HIS:NE2	1:D:2246:ARG:HG3	2.29	0.47
1:E:3331:GLU:HA	1:E:3331:GLU:OE1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:3752:ASP:OD1	1:F:3755:ILE:N	2.45	0.47
1:F:3786:GLN:HB3	1:F:3793:VAL:HB	1.95	0.47
1:F:3889:ILE:HG22	1:F:3890:MET:N	2.29	0.47
1:H:5039:VAL:HG23	1:H:5064:ILE:CG2	2.45	0.47
1:A:238:MET:HE1	1:A:464:LEU:HD22	1.95	0.47
1:C:1277:HIS:NE2	5:C:1735:ATP:H3'	2.29	0.47
1:C:1318:ILE:HG22	1:C:1408:VAL:HB	1.95	0.47
1:C:1417:LEU:HB3	1:C:1418:PRO:HD2	1.95	0.47
1:E:3100:ASP:C	1:E:3102:ILE:H	2.18	0.47
1:E:3108:ALA:HB2	1:E:3460:ARG:O	2.13	0.47
1:F:3916:CYS:HB3	1:F:3921:LYS:O	2.15	0.47
1:G:4322:LEU:HA	1:G:4404:SER:HB3	1.95	0.47
1:H:5188:MET:CE	1:H:5190:HIS:NE2	2.78	0.47
1:A:283:LEU:HD22	1:A:283:LEU:C	2.33	0.47
1:A:454:ARG:HG2	1:A:473:CYS:O	2.15	0.47
1:B:762:ASN:ND2	6:B:6065:HOH:O	2.47	0.47
1:C:1356:LEU:HD12	1:C:1357:TRP:N	2.30	0.47
1:C:1252:PRO:HG3	5:C:1735:ATP:C2	2.50	0.47
1:E:3478:GLN:HB2	1:E:3484:ASP:CB	2.44	0.47
1:F:3893:ARG:HD3	1:F:3926:ALA:O	2.14	0.47
1:H:5067:ILE:HD12	1:H:5088:GLY:HA3	1.97	0.47
1:A:515:ARG:HB3	1:A:516:PRO:HD2	1.97	0.47
1:E:3050:ILE:HD11	1:E:3068:MET:HE1	1.95	0.47
1:F:3988:MET:SD	1:F:4066:ARG:NH2	2.88	0.47
1:A:123:ILE:HD11	1:A:202:LEU:CG	2.45	0.47
1:A:334:ILE:HG12	1:A:362:GLY:O	2.15	0.47
1:A:407:LEU:HA	1:A:407:LEU:HD12	1.39	0.47
1:A:79:THR:H	1:A:82:TYR:HB3	1.78	0.47
1:C:1313:THR:O	1:C:1442:SER:OG	2.31	0.47
1:C:1320:THR:HG22	1:C:1358:LEU:CD1	2.44	0.47
1:C:1345:ASN:HD21	1:C:1361:LYS:HZ1	1.63	0.47
1:C:1376:ASP:N	1:C:1407:GLY:O	2.46	0.47
1:G:4471:GLU:O	1:G:4499:GLU:HG3	2.14	0.47
1:G:4686:ASP:O	1:G:4690:ASN:HB2	2.15	0.47
1:H:5090:MET:HE2	1:H:5126:ALA:HB3	1.96	0.47
1:H:5135:LYS:HB2	6:H:6479:HOH:O	2.14	0.47
1:B:675:PHE:CD1	1:B:711:LEU:HG	2.50	0.47
1:B:774:TYR:CE2	1:B:811:PRO:HG3	2.50	0.47
1:D:1859:THR:O	1:D:1862:GLU:N	2.47	0.47
1:E:3113:THR:HG23	1:E:3114:LYS:N	2.29	0.47
1:E:3252:GLU:HG2	6:E:7072:HOH:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3425:ALA:HB1	1:E:3502:PHE:HB3	1.97	0.47
1:F:3646:ILE:HG23	1:F:3977:GLN:NE2	2.30	0.47
1:F:3629:MET:O	1:H:5111:MET:HA	2.14	0.47
1:B:772:LYS:HE2	1:B:783:GLN:HG3	1.97	0.47
1:C:1650:ILE:HD13	1:C:1650:ILE:N	2.29	0.47
1:C:1681:TRP:CZ2	1:C:1716:PRO:HA	2.50	0.47
1:D:1945:ASN:ND2	1:D:1961:LYS:NZ	2.57	0.47
1:D:2088:GLY:O	1:D:2089:ILE:HD13	2.15	0.47
1:E:3304:LYS:O	1:E:3307:LEU:HB2	2.14	0.47
1:F:3872:ASN:ND2	1:F:3875:GLY:H	2.12	0.47
1:F:4055:ASN:O	1:F:4058:THR:HB	2.15	0.47
1:G:4222:ALA:HB1	1:G:4227:GLU:HG2	1.96	0.47
1:G:4339:LEU:CD1	1:G:4354:ASN:HA	2.43	0.47
1:G:4501:PRO:HG2	1:G:4504:LYS:HD2	1.96	0.47
1:A:172:LYS:HA	1:A:182:LEU:O	2.15	0.47
1:A:338:ARG:HG3	1:A:338:ARG:NH1	2.30	0.47
1:A:79:THR:HG1	1:A:81:GLU:HB3	1.80	0.47
1:B:976:MET:HE2	1:B:980:ILE:CD1	2.42	0.47
1:D:1812:ILE:HD13	1:D:1833:ASP:OD2	2.14	0.47
1:D:1873:MET:CE	1:D:1886:THR:HG22	2.45	0.47
1:D:2206:ASP:HB3	1:D:2209:GLU:HB2	1.96	0.47
1:D:2291:LEU:O	1:D:2291:LEU:HD12	2.14	0.47
1:E:3142:THR:HG21	1:E:3144:ASP:CB	2.45	0.47
1:F:3663:MET:CE	1:F:3668:MET:HE3	2.45	0.47
1:F:3675:PHE:CZ	1:F:3683:HIS:CD2	3.03	0.47
1:G:4417:LEU:HD12	1:G:4417:LEU:HA	1.51	0.47
1:B:660:LEU:HB3	1:B:693:ALA:CB	2.45	0.47
1:D:2127:THR:O	1:D:2128:GLN:HB2	2.14	0.47
1:E:3343:GLU:O	1:E:3347:VAL:HG23	2.15	0.47
1:F:3679:THR:OG1	1:F:3681:GLU:N	2.47	0.47
1:F:3665:LYS:HE2	1:F:3697:PHE:HE2	1.80	0.47
1:F:3889:ILE:CG2	1:F:3890:MET:N	2.78	0.47
1:G:4385:LYS:HB2	1:G:4393:VAL:O	2.15	0.47
1:C:1452:GLU:HG2	1:C:1455:LYS:NZ	2.30	0.46
1:D:1976:ASP:HB2	1:D:2006:LYS:HG3	1.98	0.46
1:D:2295:VAL:O	1:D:2299:ARG:HG3	2.16	0.46
1:E:3019:ALA:CB	1:E:3031:ARG:HB2	2.45	0.46
1:E:3055:ARG:NH2	1:E:3082:TYR:O	2.47	0.46
1:F:3659:THR:O	1:F:3663:MET:HG2	2.15	0.46
1:G:4321:GLY:N	1:G:4357:TRP:O	2.48	0.46
1:H:5327:VAL:CG1	1:H:5328:PRO:HD2	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1319:ARG:HB2	1:C:1359:ASP:OD2	2.15	0.46
1:G:4322:LEU:HD22	1:G:4326:SER:C	2.36	0.46
1:G:4560:LEU:HA	1:G:4560:LEU:HD23	1.79	0.46
1:H:4922:LEU:HB3	1:H:4926:SER:O	2.15	0.46
1:F:3928:GLN:HE21	1:H:5140:THR:HB	1.79	0.46
1:C:1591:ARG:O	1:C:1595:GLU:HG3	2.15	0.46
1:E:3382:ARG:NH1	6:E:6629:HOH:O	2.47	0.46
1:E:3425:ALA:O	1:E:3426:ALA:HB2	2.15	0.46
1:E:3402:SER:HB2	1:F:3621:MET:CE	2.45	0.46
1:G:4323:ILE:HA	1:G:4351:CYS:HB2	1.98	0.46
1:H:4860:LEU:O	1:H:4863:MET:HB2	2.15	0.46
1:A:163:ILE:CG2	1:A:163:ILE:O	2.52	0.46
1:A:439:GLN:O	1:A:442:ARG:HG2	2.15	0.46
1:B:731:VAL:HG12	1:B:732:GLU:N	2.31	0.46
1:B:739:LEU:HD12	1:B:754:ASN:O	2.14	0.46
1:B:774:TYR:HB2	1:B:809:ASN:HB2	1.98	0.46
1:B:890:MET:HE2	1:B:892:ALA:CB	2.43	0.46
1:C:1253:ALA:HB1	6:C:7310:HOH:O	2.14	0.46
1:E:3055:ARG:NH2	1:E:3085:GLU:HB3	2.31	0.46
1:F:3650:ILE:HB	1:F:3673:MET:HE1	1.98	0.46
1:G:4428:LEU:HD12	1:G:4456:ILE:HG21	1.95	0.46
1:A:24:THR:HB	1:C:1596:GLU:CD	2.35	0.46
1:A:289:ILE:CG2	1:A:290:MET:N	2.78	0.46
1:C:1257:VAL:HG12	1:C:1258:GLU:N	2.31	0.46
1:C:1263:MET:HA	1:C:1266:SER:HB2	1.97	0.46
1:C:1707:VAL:HG12	1:C:1708:VAL:N	2.31	0.46
1:D:2209:GLU:O	1:D:2213:MET:HG3	2.16	0.46
1:G:4379:LEU:C	1:G:4379:LEU:HD12	2.35	0.46
1:G:4409:ASN:ND2	6:G:6819:HOH:O	2.40	0.46
1:H:5231:THR:HG21	1:H:5234:GLY:HA2	1.97	0.46
1:H:5256:HIS:CD2	1:H:5256:HIS:H	2.34	0.46
1:A:114:LYS:HB2	6:A:6007:HOH:O	2.14	0.46
1:B:815:VAL:CB	1:B:817:LEU:HD12	2.38	0.46
6:A:7662:HOH:O	1:C:1536:LYS:HE2	2.15	0.46
1:C:1524:ILE:HG12	1:C:1557:CYS:HB2	1.96	0.46
1:D:2089:ILE:CG2	1:D:2090:MET:N	2.79	0.46
1:F:3809:ASN:C	1:F:3811:PRO:HD3	2.36	0.46
1:F:3906:PHE:HB2	6:F:6288:HOH:O	2.15	0.46
1:F:3926:ALA:HB1	1:F:3959:MET:HE2	1.97	0.46
1:F:4009:GLU:OE2	1:F:4043:TYR:OH	2.28	0.46
1:F:4080:ALA:O	1:F:4083:GLU:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4569:TYR:HB3	1:G:4572:GLU:HB2	1.97	0.46
1:H:4824:THR:OG1	1:H:4827:GLU:HB2	2.15	0.46
1:A:203:GLY:HA3	1:A:206:LYS:CE	2.45	0.46
1:A:310:LYS:HB3	1:C:1229:MET:HE2	1.98	0.46
1:B:1106:ASP:O	1:B:1129:VAL:HG23	2.16	0.46
1:C:1529:MET:O	1:C:1543:GLU:HB3	2.15	0.46
1:D:1884:ALA:HB2	1:D:2030:PHE:HZ	1.80	0.46
1:E:3220:VAL:HG11	1:E:3225:ILE:HD11	1.98	0.46
1:E:3333:MET:SD	1:E:3339:PRO:HD3	2.56	0.46
1:F:3763:ILE:HG23	1:F:3764:CYS:N	2.31	0.46
1:G:4410:LEU:CD1	1:G:4410:LEU:N	2.79	0.46
1:G:4494:GLY:HA3	1:G:4527:THR:HG21	1.96	0.46
1:G:4628:ILE:HD13	1:G:4692:ALA:HB3	1.98	0.46
1:A:131:VAL:HG22	6:A:7655:HOH:O	2.15	0.46
1:A:423:LEU:HA	1:A:423:LEU:HD12	1.74	0.46
1:B:1109:ILE:HD13	1:B:1126:VAL:HG22	1.91	0.46
1:B:698:ALA:HA	1:B:704:TYR:CD1	2.51	0.46
1:C:1226:LEU:O	1:C:1229:MET:HB2	2.16	0.46
1:C:1260:LEU:HD13	1:C:1290:VAL:HA	1.97	0.46
1:D:2038:MET:HE2	1:D:2264:LEU:HD11	1.98	0.46
1:D:2068:SER:OG	1:D:2086:SER:OG	2.28	0.46
1:E:3306:PHE:HB2	6:E:7081:HOH:O	2.14	0.46
1:F:3641:ALA:CB	1:F:4048:PRO:HG3	2.46	0.46
1:G:4593:LEU:HG	1:G:4597:LEU:HD22	1.97	0.46
1:G:4611:MET:HE1	1:G:4724:MET:HB2	1.98	0.46
1:H:5265:TYR:N	1:H:5265:TYR:CD1	2.84	0.46
1:A:162:ASN:ND2	1:A:165:LYS:HD3	2.31	0.46
1:A:432:GLU:OE1	1:A:454:ARG:HB2	2.15	0.46
1:C:1456:ILE:N	1:C:1456:ILE:CD1	2.79	0.46
1:D:2103:GLU:OE1	1:D:2103:GLU:N	2.38	0.46
1:B:949:ASN:HD21	1:D:2110:LYS:NZ	2.14	0.46
1:D:2176:MET:O	1:D:2180:ILE:HG13	2.16	0.46
1:E:3116:PRO:HD2	1:E:3243:PHE:HB2	1.97	0.46
1:E:3311:MET:SD	1:E:3315:ARG:HD3	2.56	0.46
1:E:3398:ALA:CB	1:E:3413:MET:HE1	2.46	0.46
1:A:252:GLU:O	1:A:255:LYS:HB3	2.16	0.46
1:D:1922:LEU:O	1:D:1951:CYS:HB2	2.16	0.46
1:D:2054:ARG:HD2	1:D:2066:ILE:HD12	1.97	0.46
1:E:3103:LEU:HD12	1:E:3103:LEU:HA	1.48	0.46
1:E:3172:LYS:HE3	1:E:3183:GLN:CB	2.42	0.46
1:E:3173:VAL:HB	1:E:3182:LEU:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3167:VAL:O	1:E:3187:LYS:HE3	2.16	0.46
1:F:3649:THR:HG22	1:F:3965:ALA:HB2	1.97	0.46
1:F:3929:MET:O	1:F:3943:GLU:HG2	2.15	0.46
1:A:141:ILE:HG23	1:A:156:LEU:O	2.17	0.45
1:A:118:ILE:HG21	1:A:208:VAL:HB	1.95	0.45
1:C:1250:ILE:CB	1:C:1273:MET:HE3	2.38	0.45
1:C:1335:LYS:CG	1:C:1336:GLY:N	2.79	0.45
1:C:1339:LEU:HD12	1:C:1354:ASN:O	2.16	0.45
1:C:1381:SER:O	1:C:1397:GLU:HB3	2.16	0.45
1:E:3188:GLY:HA3	1:E:3191:PHE:CD1	2.51	0.45
1:H:4889:ASN:ND2	6:H:6193:HOH:O	2.48	0.45
1:A:471:VAL:O	1:A:471:VAL:HG12	2.16	0.45
1:B:815:VAL:HG21	1:B:843:PHE:CE2	2.52	0.45
1:C:1655:ASN:HB3	1:C:1658:THR:HB	1.99	0.45
1:E:3168:ASP:O	1:E:3171:SER:HB2	2.15	0.45
1:E:3333:MET:O	1:E:3369:TYR:HB2	2.16	0.45
1:G:4376:ASP:OD2	1:G:4406:LYS:HD2	2.16	0.45
1:A:79:THR:OG1	1:A:81:GLU:HB3	2.15	0.45
1:B:1101:PHE:CD1	1:B:1101:PHE:N	2.84	0.45
1:B:1114:TRP:CD1	1:B:1115:ARG:CD	2.99	0.45
1:B:731:VAL:HG11	1:B:753:GLU:HB3	1.97	0.45
1:C:1352:ASP:OD1	1:C:1354:ASN:HB2	2.16	0.45
1:D:2188:MET:CE	1:D:2266:ARG:HH21	2.28	0.45
1:E:3350:ALA:O	1:E:3353:ASP:HB2	2.15	0.45
1:E:3465:TYR:CD1	1:E:3465:TYR:N	2.83	0.45
1:F:3721:GLY:CA	1:F:3757:TRP:CE3	2.99	0.45
1:G:4348:MET:HA	1:G:4357:TRP:CE3	2.51	0.45
1:H:4918:ILE:CD1	1:H:5010:LEU:HD22	2.46	0.45
1:H:5230:LEU:HG	1:H:5312:THR:HG22	1.98	0.45
1:H:5231:THR:O	1:H:5253:THR:HB	2.16	0.45
1:B:704:TYR:HD2	6:B:6584:HOH:O	1.99	0.45
1:C:1275:PHE:N	1:C:1275:PHE:CD1	2.83	0.45
1:C:1526:ALA:HB1	1:C:1559:MET:HE1	1.95	0.45
1:D:2090:MET:HE1	3:D:2333:OXL:O1	2.16	0.45
1:H:4926:SER:HB3	1:H:4929:ALA:N	2.21	0.45
1:H:5046:LYS:O	1:H:5049:ASP:HB2	2.16	0.45
1:H:5226:ALA:HA	1:H:5247:ALA:HB1	1.98	0.45
1:H:5244:ARG:NE	6:H:6931:HOH:O	2.42	0.45
1:A:328:GLN:NE2	1:C:1540:THR:CA	2.80	0.45
1:B:619:ALA:HB2	1:B:631:ARG:HB3	1.98	0.45
1:B:731:VAL:CG1	1:B:732:GLU:N	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1250:ILE:HG12	1:C:1271:ALA:HB1	1.97	0.45
1:C:1347:TYR:CE2	1:C:1355:ILE:CD1	3.00	0.45
1:C:1406:LYS:HD2	1:C:1406:LYS:HA	1.47	0.45
1:A:29:MET:CE	1:C:1510:LYS:HB3	2.47	0.45
1:F:4057:GLN:O	1:F:4061:GLN:HG3	2.15	0.45
1:G:4377:ASP:C	1:G:4498:ILE:HD12	2.36	0.45
1:A:333:MET:HA	1:A:336:LYS:O	2.16	0.45
1:A:63:MET:HG3	1:A:371:LEU:CD2	2.47	0.45
1:B:843:PHE:CD2	1:B:845:ARG:NE	2.85	0.45
1:C:1212:ILE:O	1:C:1212:ILE:HG22	2.15	0.45
1:A:341:ARG:H	1:C:1528:GLN:NE2	2.14	0.45
1:C:1677:VAL:HG12	1:C:1678:GLN:N	2.32	0.45
1:D:2188:MET:SD	1:D:2266:ARG:NH2	2.89	0.45
1:E:3156:LEU:HD23	1:E:3156:LEU:HA	1.70	0.45
1:A:245:ARG:HE	1:A:245:ARG:HB2	1.50	0.45
1:A:316:CYS:O	1:A:320:GLY:N	2.50	0.45
1:A:55:ARG:NH2	1:A:85:GLU:HB3	2.31	0.45
1:C:1597:LEU:HA	1:C:1597:LEU:HD12	1.68	0.45
1:C:1656:HIS:HB3	1:C:1660:ARG:NH2	2.32	0.45
1:D:1874:ASN:OD1	1:D:1876:SER:HB2	2.16	0.45
1:E:3162:ASN:HD21	1:E:3165:LYS:HE2	1.81	0.45
1:F:3676:SER:HA	1:F:3714:LYS:HG3	1.97	0.45
1:G:4342:THR:HG21	1:G:4347:TYR:HD2	1.79	0.45
1:H:5023:LYS:HG2	1:H:5027:ASP:OD2	2.17	0.45
1:A:113:THR:HG23	1:A:114:LYS:N	2.32	0.45
1:A:133:LEU:N	1:A:133:LEU:CD1	2.79	0.45
1:B:672:ARG:HD3	1:B:672:ARG:HH11	1.67	0.45
1:C:1472:ASN:O	1:C:1476:VAL:HG23	2.17	0.45
1:D:1878:GLY:HA2	6:D:6136:HOH:O	2.16	0.45
1:F:3824:ASP:O	1:F:3827:ASP:HB2	2.17	0.45
1:F:3829:LYS:CE	1:F:3856:ILE:HG23	2.46	0.45
1:F:3897:GLY:HA2	1:F:3905:VAL:CG2	2.47	0.45
1:F:3894:GLY:HA3	1:F:3927:THR:HG21	1.98	0.45
1:F:3893:ARG:NH2	1:F:3946:ASP:OD1	2.50	0.45
1:E:3340:THR:HB	1:G:4528:GLN:HE21	1.81	0.45
1:H:4990:ASP:OD1	1:H:4991:PHE:HD2	2.00	0.45
1:A:140:LYS:HE2	1:A:191:PHE:HB2	1.98	0.45
1:A:192:LEU:N	1:A:192:LEU:CD2	2.76	0.45
1:A:452:VAL:HG11	1:A:488:ARG:HB3	1.98	0.45
1:B:1104:LYS:HA	1:B:1129:VAL:HG12	1.97	0.45
1:B:640:THR:O	1:B:982:ARG:NH1	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:857:LEU:HD12	1:B:866:ILE:HD11	1.99	0.45
1:B:997:LEU:O	1:B:1000:SER:OG	2.29	0.45
1:C:1395:GLU:HB2	6:C:7744:HOH:O	2.16	0.45
1:C:1518:ARG:HB3	6:C:6442:HOH:O	2.16	0.45
1:C:1539:PRO:HG3	1:C:1576:MET:HG2	1.98	0.45
1:D:1814:THR:CG2	1:D:1815:GLN:N	2.80	0.45
1:D:1856:SER:O	1:D:1860:LEU:HB2	2.17	0.45
1:E:3049:THR:HA	1:E:3072:ARG:O	2.17	0.45
1:E:3379:LEU:HD12	1:E:3379:LEU:HA	1.85	0.45
1:F:3806:LYS:HA	1:F:3806:LYS:HD2	1.59	0.45
1:G:4212:ILE:HG22	1:G:4213:GLN:O	2.17	0.45
1:F:3941:ARG:NE	1:H:5093:ARG:O	2.50	0.45
1:H:5242:ARG:NH2	6:H:7238:HOH:O	2.29	0.45
1:A:156:LEU:CD2	1:A:157:TRP:N	2.80	0.45
1:A:48:CYS:SG	1:A:68:MET:HE2	2.57	0.45
1:B:1115:ARG:HB3	1:B:1116:PRO:HD3	1.98	0.45
1:C:1322:LEU:CD1	1:C:1349:GLU:HG2	2.35	0.45
1:C:1351:CYS:O	1:C:1352:ASP:HB3	2.17	0.45
1:C:1373:VAL:HG13	1:C:1410:LEU:HD11	1.99	0.45
1:C:1639:GLN:OE1	1:C:1642:ARG:HD3	2.16	0.45
1:C:1704:LYS:HD2	1:C:1730:PRO:O	2.17	0.45
1:D:2025:ILE:HD12	1:D:2056:ILE:HG13	1.98	0.45
1:D:2175:ARG:HG3	1:D:2175:ARG:H	1.43	0.45
1:D:2205:THR:HG23	1:D:2205:THR:O	2.17	0.45
1:E:3012:ILE:CG2	1:E:3013:GLN:N	2.79	0.45
1:F:3837:ASP:HB3	1:F:4061:GLN:HG2	1.99	0.45
1:F:3878:ARG:O	1:F:3881:GLU:HG2	2.16	0.45
1:F:3922:PRO:HB3	1:F:4064:LEU:O	2.17	0.45
1:G:4255:ARG:NE	1:G:4282:TYR:CZ	2.85	0.45
1:H:4960:TYR:CD2	1:H:4963:ILE:HB	2.52	0.45
1:H:4960:TYR:OH	1:H:5016:ASP:HB2	2.16	0.45
1:G:4221:MET:HE1	1:H:5202:SER:HB2	1.99	0.45
1:G:4613:MET:SD	1:H:5221:LYS:HE2	2.57	0.45
1:A:131:VAL:HG13	1:A:133:LEU:CD1	2.47	0.44
1:A:158:LEU:HA	1:A:158:LEU:HD12	1.41	0.44
1:A:242:SER:HA	1:A:269:LYS:HB2	1.98	0.44
1:A:300:ILE:HB	1:A:301:PRO:CD	2.48	0.44
1:A:293:ARG:NH2	1:A:346:ASP:OD1	2.44	0.44
1:B:1030:LEU:N	1:B:1030:LEU:HD12	2.32	0.44
1:B:655:ARG:HD2	1:B:682:TYR:OH	2.17	0.44
1:D:1841:ALA:CB	1:D:2248:PRO:HG3	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1863:MET:HE2	1:D:2174:VAL:HG21	1.99	0.44
1:F:3719:ARG:HD3	1:F:3807:GLY:HA2	1.99	0.44
1:A:267:ILE:N	1:A:267:ILE:CD1	2.79	0.44
1:C:1287:ILE:CG2	1:C:1291:ARG:NH1	2.80	0.44
1:C:1482:ILE:O	1:C:1486:SER:OG	2.34	0.44
1:C:1664:LEU:HD12	1:C:1664:LEU:HA	1.77	0.44
1:D:1855:ARG:HD2	1:D:1882:TYR:CZ	2.52	0.44
1:E:3328:GLN:NE2	1:G:4540:THR:HA	2.30	0.44
1:G:4303:LEU:HA	1:G:4303:LEU:HD22	1.78	0.44
1:F:3941:ARG:N	1:H:5128:GLN:NE2	2.55	0.44
1:H:5285:VAL:O	1:H:5289:VAL:HG23	2.17	0.44
1:A:52:PRO:HD2	1:A:365:ALA:O	2.17	0.44
1:A:481:TRP:HB2	1:A:516:PRO:HG3	2.00	0.44
1:B:1129:VAL:HA	1:B:1130:PRO:HD2	1.71	0.44
1:B:724:LYS:HE2	1:B:752:ASP:HB3	2.00	0.44
1:C:1425:ILE:O	1:C:1428:LEU:HB2	2.18	0.44
1:C:1611:MET:HE3	1:C:1724:MET:HB2	1.98	0.44
1:E:3126:SER:HB3	1:E:3129:ALA:CB	2.46	0.44
1:E:3209:ASN:O	1:E:3210:LEU:HD23	2.17	0.44
1:E:3453:THR:HG21	1:E:3459:ALA:HB2	2.00	0.44
1:E:3456:HIS:H	1:E:3456:HIS:CD2	2.35	0.44
1:F:3695:GLU:HA	1:F:3695:GLU:OE1	2.16	0.44
1:F:3700:ASP:HA	1:F:3701:PRO:HD2	1.83	0.44
1:F:3774:TYR:CE2	1:F:3811:PRO:HG2	2.52	0.44
1:F:3838:MET:HA	1:F:3864:ILE:CG2	2.46	0.44
1:F:3890:MET:CE	1:F:3892:ALA:HB2	2.46	0.44
1:F:4031:THR:HG21	1:F:4034:GLY:HA2	1.99	0.44
1:A:130:GLU:HG3	1:A:201:PHE:HB3	1.99	0.44
1:A:406:ASP:OD1	1:A:407:LEU:N	2.51	0.44
1:A:503:LYS:O	1:A:529:VAL:HB	2.18	0.44
1:B:975:ARG:O	1:B:978:HIS:HB3	2.17	0.44
1:C:1356:LEU:C	1:C:1356:LEU:HD12	2.38	0.44
1:D:1959:ASP:HB3	6:D:7764:HOH:O	2.18	0.44
1:E:3245:ARG:HB3	1:E:3274:GLU:CG	2.38	0.44
1:E:3469:PHE:N	1:E:3469:PHE:CD1	2.86	0.44
1:F:3687:ILE:O	1:F:3691:ARG:HG3	2.18	0.44
1:F:3890:MET:HE1	1:F:3892:ALA:CB	2.46	0.44
1:E:3293:ARG:HB3	1:G:4541:ARG:HG3	1.98	0.44
1:G:4711:LEU:HB3	1:G:4721:THR:OG1	2.17	0.44
1:H:4931:VAL:HG12	1:H:4932:GLU:H	1.82	0.44
1:A:209:ASN:HB3	1:A:299:GLU:OE2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1028:ILE:HG13	1:B:1108:VAL:HG11	2.00	0.44
1:B:647:ILE:HG12	1:B:670:VAL:HB	2.00	0.44
1:B:748:MET:HB2	1:B:757:TRP:CD2	2.52	0.44
1:C:1250:ILE:HG21	1:C:1286:THR:CG2	2.47	0.44
1:C:1283:HIS:O	1:C:1287:ILE:HG12	2.18	0.44
1:C:1276:SER:HB3	1:C:1319:ARG:HD2	2.00	0.44
1:D:1887:ILE:CG2	1:D:1891:ARG:NH1	2.80	0.44
1:D:2044:ILE:CG1	1:D:2068:SER:HB3	2.44	0.44
1:D:2192:LYS:HD2	6:D:7514:HOH:O	2.16	0.44
1:E:3205:LYS:HG2	6:E:6937:HOH:O	2.18	0.44
1:F:3713:THR:HG22	1:F:3842:SER:HB2	1.99	0.44
1:F:4105:GLY:N	1:F:4129:VAL:O	2.40	0.44
1:G:4444:ILE:HG23	1:G:4449:ASP:HB2	1.99	0.44
1:G:4693:MET:CE	1:G:4729:VAL:HG22	2.46	0.44
1:H:4948:MET:HB2	1:H:4948:MET:HE2	1.60	0.44
1:H:5010:LEU:HB3	1:H:5013:ALA:HB3	1.99	0.44
1:B:882:ILE:O	1:B:886:SER:OG	2.31	0.44
1:C:1358:LEU:HA	1:C:1358:LEU:HD12	1.71	0.44
1:C:1445:ARG:HG2	1:C:1474:GLU:HB3	1.98	0.44
1:C:1650:ILE:CD1	1:C:1669:PHE:HB2	2.47	0.44
1:F:3842:SER:HA	1:F:3869:LYS:HD3	1.99	0.44
1:F:4032:GLU:OE1	1:F:4054:ARG:N	2.40	0.44
1:G:4363:ILE:CG2	1:G:4364:CYS:N	2.79	0.44
1:G:4368:ASP:O	1:G:4384:VAL:HG11	2.18	0.44
1:G:4631:THR:O	1:G:4653:THR:OG1	2.29	0.44
1:H:5089:ILE:CG2	1:H:5090:MET:N	2.80	0.44
1:A:277:ARG:NH2	1:A:278:ARG:CZ	2.81	0.44
1:A:338:ARG:HG3	1:A:338:ARG:HH11	1.83	0.44
1:B:935:LYS:HD2	1:B:935:LYS:HA	1.75	0.44
1:C:1287:ILE:HG22	1:C:1291:ARG:HD2	1.99	0.44
1:C:1345:ASN:HD21	1:C:1361:LYS:NZ	2.16	0.44
1:C:1534:ILE:HG23	1:C:1567:GLY:CA	2.41	0.44
1:B:904:LYS:HB3	1:D:1834:ILE:HG22	1.99	0.44
1:D:2009:ASN:C	1:D:2011:PRO:HD3	2.37	0.44
1:F:3735:LYS:HG2	1:F:3736:GLY:N	2.33	0.44
1:H:4855:ARG:HD3	6:H:7187:HOH:O	2.18	0.44
1:H:5179:LEU:HA	1:H:5179:LEU:HD23	1.79	0.44
1:C:1341:ILE:HD12	1:C:1394:THR:CG2	2.46	0.44
1:C:1446:LYS:HE2	6:C:7626:HOH:O	2.18	0.44
1:C:1457:LEU:HD23	1:C:1466:ILE:HD11	2.00	0.44
1:D:2009:ASN:C	1:D:2010:LEU:HD22	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2030:PHE:CE1	1:D:2034:GLN:CG	3.00	0.44
1:D:2126:ALA:O	1:D:2127:THR:HB	2.18	0.44
1:E:3114:LYS:HD3	6:E:6705:HOH:O	2.17	0.44
1:E:3294:GLY:HA3	1:E:3327:THR:HG21	2.00	0.44
1:F:4029:VAL:O	1:F:4051:ALA:HA	2.18	0.44
1:G:4319:ARG:O	1:G:4359:ASP:HB2	2.16	0.44
1:G:4337:ALA:O	1:G:4396:VAL:N	2.34	0.44
1:G:4628:ILE:HD13	1:G:4692:ALA:HB1	1.98	0.44
1:G:4652:VAL:CG2	1:G:4692:ALA:HB2	2.47	0.44
1:H:4847:ILE:CG2	1:H:5159:MET:HE2	2.45	0.44
1:A:47:ILE:CB	1:A:359:MET:HG3	2.48	0.44
1:B:843:PHE:CE2	1:B:845:ARG:HD3	2.52	0.44
1:B:890:MET:HE3	1:B:892:ALA:HA	2.00	0.44
1:B:992:LYS:O	1:B:996:GLU:HG3	2.18	0.44
1:C:1699:ARG:HD3	1:C:1701:PHE:CE2	2.53	0.44
1:F:3872:ASN:ND2	6:F:6201:HOH:O	2.50	0.44
1:G:4364:CYS:O	1:G:4387:LYS:HE3	2.17	0.44
1:B:738:THR:CG2	1:B:739:LEU:N	2.79	0.43
1:B:988:MET:SD	1:B:1066:ARG:NH2	2.91	0.43
1:D:2320:PHE:CE2	1:D:2322:ASN:HB3	2.53	0.43
1:E:3220:VAL:CG1	1:E:3225:ILE:HD13	2.46	0.43
1:H:4843:ASN:H	1:H:5185:GLU:CD	2.22	0.43
1:H:5038:MET:HE2	1:H:5264:LEU:HD22	2.00	0.43
1:B:1061:GLN:O	1:B:1064:LEU:HB2	2.18	0.43
1:B:1078:GLN:NE2	1:B:1078:GLN:CA	2.79	0.43
1:B:637:ALA:HA	1:B:638:PRO:HD3	1.79	0.43
1:C:1679:GLU:HG3	1:C:1680:ALA:N	2.32	0.43
1:D:1914:LYS:HD3	6:D:7805:HOH:O	2.17	0.43
1:E:3113:THR:CG2	1:E:3242:SER:H	2.30	0.43
1:E:3278:ARG:O	1:E:3282:ILE:HG13	2.19	0.43
1:G:4302:ILE:HD12	1:G:4694:ASN:HB3	2.00	0.43
1:H:4931:VAL:HG12	1:H:4932:GLU:N	2.33	0.43
1:H:5049:ASP:O	1:H:5053:VAL:HG23	2.18	0.43
1:A:246:LYS:CG	1:A:248:ALA:HB3	2.46	0.43
1:D:2020:VAL:HG11	1:D:2025:ILE:HD11	1.99	0.43
1:F:3842:SER:HB3	1:F:3843:PHE:CD2	2.53	0.43
1:F:3931:GLU:O	1:F:3934:ILE:HG13	2.18	0.43
1:G:4250:ILE:CG1	1:G:4273:MET:HE1	2.47	0.43
1:G:4322:LEU:HD21	1:G:4327:GLY:HA2	1.99	0.43
1:G:4387:LYS:HA	1:G:4392:LEU:CD1	2.48	0.43
1:G:4552:LEU:HD12	1:G:4552:LEU:HA	1.70	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:5237:ALA:HB1	1:H:5268:ILE:HD13	2.00	0.43
1:A:176:ASP:HB3	1:A:179:LEU:CB	2.48	0.43
1:A:221:SER:CB	1:A:224:ASP:H	2.25	0.43
1:D:2192:LYS:HE3	1:D:2196:GLU:OE2	2.18	0.43
1:E:3253:VAL:HG12	1:E:3257:LEU:HD23	1.96	0.43
1:E:3300:ILE:HB	1:E:3301:PRO:CD	2.49	0.43
1:E:3366:LYS:HG2	5:E:3535:ATP:H1'	2.00	0.43
1:F:3717:GLU:OE2	1:F:3719:ARG:NE	2.49	0.43
1:A:132:GLU:HA	1:A:201:PHE:HA	2.01	0.43
1:B:779:LEU:HD23	1:B:779:LEU:HA	1.69	0.43
1:B:825:ILE:O	1:B:829:LYS:HG3	2.19	0.43
1:C:1636:SER:O	1:C:1640:VAL:HG23	2.18	0.43
1:D:1874:ASN:HA	1:D:1912:ASP:HB3	2.00	0.43
1:D:2017:LEU:HB3	1:D:2018:PRO:HD2	2.00	0.43
1:B:941:ARG:HG2	1:D:2128:GLN:NE2	2.33	0.43
1:E:3013:GLN:HB3	1:E:3014:THR:H	1.54	0.43
1:F:3732:GLU:HA	1:F:3800:GLY:O	2.18	0.43
1:F:4065:TYR:CD1	1:F:4065:TYR:N	2.85	0.43
1:G:4316:PRO:HG2	1:G:4443:PHE:CB	2.49	0.43
1:H:5072:ASN:ND2	1:H:5075:GLY:H	2.16	0.43
1:H:5275:ASP:OD2	1:H:5287:LEU:HD21	2.18	0.43
1:A:464:LEU:HA	1:A:464:LEU:HD13	1.68	0.43
1:C:1274:ASN:O	1:C:1283:HIS:NE2	2.51	0.43
1:D:1855:ARG:NH2	1:D:1885:GLU:CG	2.80	0.43
1:F:3723:ILE:H	1:F:3723:ILE:HG12	1.53	0.43
1:H:4986:GLN:HG2	1:H:4993:VAL:CG2	2.49	0.43
1:F:3910:LYS:HZ1	1:H:5149:ASN:HD21	1.65	0.43
1:H:5256:HIS:O	1:H:5260:ARG:HG3	2.19	0.43
1:A:181:SER:O	1:A:197:GLU:HB2	2.18	0.43
1:C:1494:GLY:CA	1:C:1527:THR:HG21	2.48	0.43
1:C:1239:ILE:O	1:C:1582:ARG:HD3	2.19	0.43
1:D:1968:ASP:O	1:D:1971:SER:HB2	2.18	0.43
1:D:2020:VAL:HG11	1:D:2025:ILE:CD1	2.49	0.43
1:E:3144:ASP:HB3	1:E:3147:TYR:CD2	2.51	0.43
1:E:3244:ILE:HD13	1:E:3244:ILE:HA	1.78	0.43
1:E:3266:ILE:HG21	1:E:3266:ILE:HD13	1.72	0.43
1:F:3867:ILE:HA	1:F:3888:GLY:O	2.18	0.43
1:G:4640:VAL:CG1	1:G:4649:ILE:HD13	2.49	0.43
1:A:181:SER:H	1:A:198:ASN:HD21	1.66	0.43
1:B:770:GLY:HA2	1:B:783:GLN:HE21	1.83	0.43
1:B:928:GLN:HE21	1:D:2141:ARG:HB2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1218:HIS:CD2	1:C:1231:ARG:HD3	2.53	0.43
1:C:1416:ASP:OD1	1:C:1416:ASP:N	2.46	0.43
1:C:1465:LYS:HA	1:C:1487:ASP:OD2	2.18	0.43
1:B:938:ARG:NH2	1:D:1978:GLY:O	2.47	0.43
1:E:3351:VAL:HG13	1:E:3466:ARG:NH2	2.34	0.43
1:F:3700:ASP:OD2	1:F:3703:LEU:HD13	2.19	0.43
1:F:3956:ASP:HB3	1:F:4064:LEU:O	2.18	0.43
1:G:4532:SER:OG	1:G:4543:GLU:OE1	2.29	0.43
1:H:4941:ILE:HA	1:H:4956:LEU:O	2.18	0.43
1:A:148:MET:HB3	1:A:148:MET:HE3	1.75	0.43
1:B:844:ILE:HG13	1:B:868:SER:CB	2.47	0.43
1:B:845:ARG:O	1:B:846:LYS:HB3	2.17	0.43
1:C:1235:ASP:HA	6:C:7739:HOH:O	2.17	0.43
1:C:1323:ILE:CG2	1:C:1324:LYS:HG3	2.45	0.43
1:C:1445:ARG:HB3	1:C:1474:GLU:CD	2.39	0.43
1:D:2094:GLY:HA3	1:D:2127:THR:HG21	2.01	0.43
1:F:3714:LYS:HG2	1:F:3717:GLU:OE1	2.18	0.43
1:F:3735:LYS:HG3	1:F:3797:GLU:O	2.19	0.43
1:G:4260:LEU:HD23	1:G:4260:LEU:HA	1.89	0.43
1:E:3341:ARG:N	1:G:4528:GLN:HE21	2.00	0.43
1:A:248:ALA:HB2	6:A:7561:HOH:O	2.19	0.43
1:B:617:LEU:O	1:B:620:ALA:HB3	2.18	0.43
1:D:1880:HIS:ND1	1:D:2030:PHE:CD2	2.87	0.43
1:B:928:GLN:HE21	1:D:2141:ARG:CB	2.32	0.43
1:E:3143:LEU:HA	1:E:3143:LEU:HD12	1.55	0.43
1:F:3642:ARG:HB2	1:F:3982:ARG:CG	2.48	0.43
1:F:3857:LEU:HD23	1:F:3857:LEU:HA	1.91	0.43
1:G:4470:ILE:HG21	1:G:4476:VAL:HG22	2.01	0.43
1:H:4941:ILE:CD1	1:H:4994:THR:HG21	2.49	0.43
1:A:425:ALA:O	1:A:448:PRO:HD2	2.19	0.42
1:A:75:PHE:CD1	1:A:75:PHE:N	2.87	0.42
1:B:719:ARG:CG	1:B:719:ARG:HH11	2.32	0.42
1:B:879:PHE:CZ	1:B:883:LEU:HG	2.54	0.42
1:C:1471:GLU:HA	1:C:1496:LEU:HB2	2.00	0.42
1:D:2047:ALA:HB2	1:D:2081:GLU:HG3	2.00	0.42
1:E:3398:ALA:HB1	1:E:3413:MET:HE1	2.00	0.42
1:G:4259:THR:O	1:G:4263:MET:HG2	2.19	0.42
1:G:4652:VAL:HA	1:G:4671:VAL:O	2.19	0.42
1:H:4966:VAL:O	6:H:7456:HOH:O	2.21	0.42
1:H:5245:PRO:CG	1:H:5249:ILE:HD11	2.48	0.42
1:A:98:ALA:HA	1:A:104:TYR:CD1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522:ASN:N	1:A:522:ASN:HD22	2.10	0.42
1:B:615:GLN:O	1:B:615:GLN:HG2	2.18	0.42
1:D:2139:PRO:HD2	6:D:7610:HOH:O	2.20	0.42
1:E:3141:ILE:HA	1:E:3156:LEU:O	2.19	0.42
1:E:3172:LYS:HA	1:E:3182:LEU:O	2.19	0.42
1:E:3172:LYS:HA	1:E:3172:LYS:HD2	1.42	0.42
1:F:3906:PHE:O	1:F:3910:LYS:HG3	2.19	0.42
1:F:4030:LEU:HD22	1:F:4052:VAL:HB	2.00	0.42
1:G:4330:GLU:HA	1:G:4402:LEU:O	2.18	0.42
1:G:4526:ALA:O	1:G:4527:THR:HB	2.19	0.42
1:A:507:VAL:CG1	1:A:508:VAL:N	2.79	0.42
1:B:615:GLN:HA	6:B:6399:HOH:O	2.19	0.42
1:B:700:ASP:OD2	1:B:703:LEU:HB2	2.19	0.42
1:B:969:TYR:HD1	1:B:972:GLU:OE1	2.02	0.42
1:D:1967:VAL:HG13	1:D:1968:ASP:N	2.34	0.42
1:D:1986:GLN:HB2	1:D:1986:GLN:HE21	1.50	0.42
1:D:2281:TRP:CG	1:D:2316:PRO:HD3	2.54	0.42
1:F:3622:ALA:O	1:F:3991:ARG:NH2	2.52	0.42
1:F:4081:TRP:O	1:F:4085:VAL:N	2.39	0.42
1:G:4409:ASN:O	1:G:4411:PRO:HD3	2.18	0.42
1:G:4522:PRO:HD3	1:G:4665:TYR:CE2	2.54	0.42
1:G:4656:HIS:N	1:G:4656:HIS:ND1	2.65	0.42
1:H:5063:ASN:HB2	6:H:7226:HOH:O	2.18	0.42
1:D:1875:PHE:CD1	1:D:1911:LEU:HG	2.54	0.42
1:D:2083:LEU:HD21	1:D:2119:ALA:HB2	2.02	0.42
1:E:3109:VAL:N	1:E:3237:ASP:OD2	2.40	0.42
1:E:3514:TRP:N	1:E:3522:ASN:OD1	2.41	0.42
1:F:3864:ILE:CG2	1:F:3865:LYS:N	2.82	0.42
1:G:4369:VAL:HA	1:G:4384:VAL:HG12	2.00	0.42
1:G:4680:ALA:HB3	1:G:4683:GLU:CD	2.40	0.42
1:H:5139:PRO:HG3	1:H:5176:MET:HG2	2.01	0.42
1:A:174:TYR:HA	1:A:180:ILE:O	2.19	0.42
1:A:246:LYS:HG3	1:A:248:ALA:CB	2.48	0.42
1:A:38:PRO:HD3	1:A:383:GLU:OE2	2.19	0.42
1:A:525:ARG:HA	1:B:1122:ASN:O	2.18	0.42
1:B:838:MET:HG3	1:B:840:PHE:CE1	2.53	0.42
1:B:926:ALA:O	1:B:927:THR:HB	2.19	0.42
1:C:1347:TYR:CE2	1:C:1355:ILE:HD12	2.55	0.42
1:D:1887:ILE:CD1	1:D:1887:ILE:N	2.79	0.42
1:D:2311:LEU:HA	1:D:2323:THR:O	2.19	0.42
1:E:3131:VAL:HG12	1:E:3202:LEU:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3133:LEU:HD12	1:E:3133:LEU:HA	1.71	0.42
1:E:3206:LYS:HE3	6:E:6233:HOH:O	2.19	0.42
1:F:3717:GLU:CD	1:F:3719:ARG:HE	2.22	0.42
1:C:1323:ILE:C	1:C:1324:LYS:HG3	2.40	0.42
1:C:1382:LEU:HD22	1:C:1394:THR:OG1	2.19	0.42
1:C:1447:ALA:HB2	1:C:1481:GLU:O	2.20	0.42
1:C:1534:ILE:HA	6:C:7028:HOH:O	2.20	0.42
1:D:2089:ILE:HG22	1:D:2090:MET:N	2.35	0.42
1:E:3115:GLY:O	1:E:3117:GLU:N	2.52	0.42
1:E:3178:GLY:HA3	1:E:3298:ILE:HD13	2.01	0.42
1:F:3764:CYS:N	6:F:7596:HOH:O	2.44	0.42
1:G:4325:GLY:N	1:G:4349:GLU:O	2.52	0.42
1:H:4923:ILE:HA	1:H:4951:CYS:O	2.19	0.42
1:H:4933:LEU:HA	1:H:4933:LEU:HD23	1.83	0.42
1:A:229:LYS:O	1:A:233:GLU:HG3	2.20	0.42
1:A:60:LEU:HA	1:A:60:LEU:HD12	1.59	0.42
1:B:640:THR:HA	1:B:982:ARG:NH1	2.34	0.42
1:B:892:ALA:O	1:B:896:LEU:HB2	2.19	0.42
1:C:1249:THR:OG1	1:C:1561:SER:HA	2.19	0.42
1:C:1320:THR:HA	1:C:1358:LEU:CD1	2.50	0.42
1:C:1503:GLU:OE1	1:C:1503:GLU:N	2.38	0.42
1:C:1703:LYS:O	1:C:1729:VAL:HB	2.20	0.42
1:D:1818:HIS:CD2	1:D:1831:ARG:HD3	2.54	0.42
1:D:1851:GLY:C	1:D:1855:ARG:HG3	2.39	0.42
1:D:2271:VAL:HG11	1:D:2291:LEU:HG	2.02	0.42
1:D:2315:ARG:CB	1:D:2316:PRO:HD2	2.47	0.42
1:E:3430:LEU:HD21	1:E:3488:ARG:HB2	2.01	0.42
1:F:3783:GLN:HG2	1:F:3784:VAL:N	2.35	0.42
1:F:4081:TRP:O	1:F:4085:VAL:HG23	2.20	0.42
1:G:4275:PHE:HB2	1:G:4312:ASP:O	2.20	0.42
1:G:4316:PRO:HG2	1:G:4443:PHE:HB2	2.01	0.42
1:G:4516:CYS:HB3	1:G:4521:LYS:O	2.19	0.42
1:G:4726:VAL:HG23	1:H:5211:MET:SD	2.60	0.42
1:A:310:LYS:NZ	1:A:353:ASP:OD1	2.53	0.42
1:C:1334:LYS:HB3	1:C:1334:LYS:HE3	1.72	0.42
1:C:1338:THR:CG2	1:C:1339:LEU:N	2.83	0.42
1:C:1457:LEU:HD12	1:C:1457:LEU:HA	1.51	0.42
1:D:2256:HIS:N	1:D:2256:HIS:CD2	2.87	0.42
1:F:3739:LEU:HG	1:F:3740:LYS:N	2.34	0.42
1:F:3774:TYR:HB3	1:F:3778:GLY:HA2	2.02	0.42
1:G:4625:ALA:O	1:G:4648:PRO:HD2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:5010:LEU:HB3	1:H:5013:ALA:CB	2.50	0.42
1:H:5193:LEU:HD21	6:H:6931:HOH:O	2.20	0.42
1:H:4841:ALA:HB2	1:H:5301:PHE:CE1	2.54	0.42
1:A:182:LEU:HD22	1:A:196:VAL:HA	2.01	0.42
1:A:493:MET:HE2	1:A:529:VAL:HG13	2.01	0.42
1:D:1985:LYS:HD3	1:D:1985:LYS:HA	1.87	0.42
1:E:3016:GLN:HG3	6:E:6528:HOH:O	2.20	0.42
1:E:3112:ASP:OD2	1:E:3269:LYS:NZ	2.48	0.42
1:E:3225:ILE:CD1	1:E:3256:ILE:HD12	2.45	0.42
1:E:3292:ALA:HB1	3:E:3533:OXL:C2	2.49	0.42
1:F:3740:LYS:O	1:F:3755:ILE:HA	2.20	0.42
1:G:4680:ALA:O	1:G:4683:GLU:HB2	2.19	0.42
1:H:4974:TYR:CD2	1:H:5011:PRO:HG3	2.55	0.42
1:H:5111:MET:O	1:H:5115:ARG:HG3	2.20	0.42
1:A:163:ILE:HG12	1:A:163:ILE:O	2.19	0.42
1:B:664:ILE:HG22	1:B:665:LYS:N	2.34	0.42
1:B:716:PRO:HG2	1:B:843:PHE:HD2	1.79	0.42
1:B:733:LEU:N	1:B:800:GLY:O	2.40	0.42
1:C:1258:GLU:O	1:C:1258:GLU:HG2	2.20	0.42
1:A:328:GLN:HE21	1:C:1540:THR:HB	1.82	0.42
1:C:1727:VAL:HA	1:C:1728:PRO:HD3	1.85	0.42
1:D:1879:THR:H	1:D:1882:TYR:HB3	1.85	0.42
1:E:3164:CYS:O	1:E:3187:LYS:HE3	2.19	0.42
1:E:3220:VAL:CG1	1:E:3225:ILE:CD1	2.95	0.42
1:F:3964:THR:HA	1:F:3970:PRO:HB3	2.01	0.42
1:G:4341:ILE:HB	1:G:4392:LEU:CB	2.46	0.42
1:G:4459:GLU:O	1:G:4459:GLU:HG3	2.20	0.42
1:G:4696:GLY:HA3	1:G:4702:PHE:CZ	2.54	0.42
1:H:5304:LYS:HA	1:H:5329:VAL:HG12	2.02	0.42
1:A:162:ASN:O	1:A:164:CYS:N	2.43	0.41
1:A:181:SER:HB3	1:A:198:ASN:ND2	2.35	0.41
1:A:294:GLY:HA3	1:A:327:THR:HG21	2.02	0.41
1:B:1035:ARG:HD3	6:B:7457:HOH:O	2.19	0.41
1:D:1911:LEU:C	1:D:1911:LEU:HD23	2.40	0.41
1:D:2020:VAL:CG1	1:D:2025:ILE:HD11	2.50	0.41
1:D:2056:ILE:HD13	1:D:2056:ILE:N	2.35	0.41
1:E:3157:TRP:CH2	1:E:3159:ASP:HB3	2.55	0.41
1:F:3735:LYS:HA	1:F:3796:VAL:HG12	2.02	0.41
1:F:3830:PHE:O	1:F:3834:GLN:N	2.45	0.41
1:G:4471:GLU:HA	1:G:4496:LEU:HB2	2.01	0.41
1:G:4696:GLY:O	1:G:4701:PHE:N	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:5244:ARG:HH11	1:H:5244:ARG:HD3	1.57	0.41
1:A:301:PRO:HG2	1:A:304:LYS:CE	2.50	0.41
1:A:431:THR:HG23	1:A:434:GLY:HA2	1.97	0.41
1:B:747:TYR:CD1	1:B:747:TYR:N	2.89	0.41
1:C:1727:VAL:HG12	1:C:1728:PRO:N	2.34	0.41
1:D:1855:ARG:HH22	1:D:1885:GLU:HG2	1.81	0.41
1:D:2008:VAL:HG12	1:D:2010:LEU:HD21	2.00	0.41
1:E:3228:LEU:CD1	1:E:3256:ILE:HG21	2.50	0.41
1:E:3289:ILE:HG22	1:E:3290:MET:N	2.35	0.41
1:F:3774:TYR:HE2	1:F:3811:PRO:HG2	1.84	0.41
1:G:4321:GLY:CA	1:G:4357:TRP:HE3	2.32	0.41
1:G:4529:MET:O	1:G:4543:GLU:HG2	2.20	0.41
1:G:4630:LEU:CD1	1:G:4712:THR:HG22	2.49	0.41
1:H:5076:VAL:O	1:H:5079:PHE:HB2	2.20	0.41
1:H:5038:MET:HE1	1:H:5264:LEU:HD22	2.02	0.41
1:H:5276:PRO:O	1:H:5278:GLN:OE1	2.38	0.41
1:A:42:ARG:HB2	1:A:378:HIS:CE1	2.55	0.41
1:B:1128:PRO:O	1:B:1130:PRO:HD3	2.20	0.41
1:B:774:TYR:HB3	1:B:778:GLY:HA2	2.03	0.41
1:G:4522:PRO:HB3	1:G:4664:LEU:O	2.20	0.41
1:A:118:ILE:HG12	1:A:160:TYR:HB2	2.01	0.41
1:A:316:CYS:SG	1:A:323:VAL:HB	2.60	0.41
1:B:655:ARG:O	1:B:660:LEU:HD22	2.20	0.41
1:C:1273:MET:HG2	1:C:1287:ILE:HD11	2.01	0.41
1:C:1285:GLU:O	1:C:1288:LYS:HB3	2.20	0.41
1:C:1472:ASN:HD21	1:C:1475:GLY:H	1.61	0.41
1:E:3220:VAL:O	1:E:3220:VAL:HG12	2.12	0.41
1:E:3507:VAL:CG1	1:E:3508:VAL:N	2.79	0.41
1:E:3402:SER:HB2	1:F:3621:MET:HE1	2.02	0.41
1:F:3672:ARG:C	1:F:3673:MET:HE3	2.40	0.41
1:F:3942:ALA:HB2	1:H:5146:ASP:OD2	2.20	0.41
1:G:4377:ASP:O	1:G:4498:ILE:HD12	2.20	0.41
1:G:4382:LEU:HA	1:G:4382:LEU:HD12	1.65	0.41
1:H:4847:ILE:CG2	1:H:5159:MET:CE	2.99	0.41
1:H:5188:MET:HE2	6:H:6225:HOH:O	2.20	0.41
1:A:228:LEU:O	1:A:232:VAL:HG23	2.20	0.41
1:A:257:LEU:HA	1:A:257:LEU:HD12	1.71	0.41
1:A:428:ILE:HD13	1:A:428:ILE:HG21	1.77	0.41
1:B:889:ILE:HG22	1:B:890:MET:N	2.36	0.41
1:C:1273:MET:CE	1:C:1286:THR:CG2	2.99	0.41
1:C:1273:MET:HE1	1:C:1286:THR:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1345:ASN:O	1:C:1347:TYR:N	2.53	0.41
1:D:1833:ASP:HB3	1:D:1836:SER:HB2	2.03	0.41
1:D:2254:ARG:NH1	1:D:2277:VAL:HG22	2.35	0.41
1:E:3493:MET:HE1	1:E:3529:VAL:CG1	2.42	0.41
1:F:3724:LYS:O	1:F:3726:SER:N	2.47	0.41
1:H:5081:GLU:HG2	6:H:6308:HOH:O	2.20	0.41
1:A:336:LYS:HA	1:A:337:PRO:HD3	1.92	0.41
1:B:1088:ARG:O	1:B:1091:LEU:HB3	2.20	0.41
1:B:618:HIS:ND1	1:B:631:ARG:HD3	2.36	0.41
1:C:1693:MET:HG2	1:C:1730:PRO:HD2	2.01	0.41
1:D:1900:ASP:OD2	1:D:1903:LEU:HG	2.21	0.41
1:D:1958:LEU:HA	1:D:1958:LEU:HD23	1.83	0.41
1:D:2065:LYS:HD3	1:D:2065:LYS:HA	1.76	0.41
1:D:2188:MET:HE2	1:D:2266:ARG:NH2	2.31	0.41
1:D:2239:GLN:O	1:D:2242:ARG:HG2	2.20	0.41
1:E:3048:CYS:SG	1:E:3068:MET:HB2	2.61	0.41
1:E:3334:ILE:HA	6:E:7083:HOH:O	2.21	0.41
1:F:3928:GLN:NE2	1:H:5140:THR:CA	2.84	0.41
1:F:3992:LYS:O	1:F:3996:GLU:HG3	2.19	0.41
1:F:3993:LEU:HD21	1:F:4044:ARG:HG3	2.02	0.41
1:G:4248:CYS:SG	1:G:4268:MET:HB2	2.61	0.41
1:G:4323:ILE:HD13	1:G:4351:CYS:CB	2.47	0.41
1:G:4609:GLU:HB3	1:H:5221:LYS:HE3	2.03	0.41
1:G:4660:ARG:HD2	1:G:4660:ARG:HH11	1.64	0.41
1:H:4941:ILE:CD1	1:H:4994:THR:CG2	2.98	0.41
1:A:29:MET:HE2	1:C:1510:LYS:HB3	2.03	0.41
1:A:57:VAL:O	1:A:57:VAL:HG12	2.20	0.41
1:B:1127:VAL:CG1	1:B:1128:PRO:N	2.82	0.41
1:C:1303:LEU:HA	1:C:1305:ARG:HH21	1.86	0.41
1:C:1483:LEU:HA	1:C:1483:LEU:HD23	1.78	0.41
1:C:1515:ARG:O	1:C:1518:ARG:HB3	2.21	0.41
1:D:1947:TYR:CD1	1:D:1947:TYR:N	2.89	0.41
1:E:3160:TYR:HD2	1:E:3163:ILE:CA	2.33	0.41
1:G:4251:GLY:O	1:G:4255:ARG:N	2.52	0.41
1:H:4843:ASN:HB3	1:H:5267:GLY:N	2.36	0.41
1:H:5090:MET:CE	1:H:5126:ALA:HB3	2.50	0.41
1:G:4621:LYS:HE2	1:H:5209:GLU:HB3	2.03	0.41
1:A:114:LYS:HG2	1:A:117:GLU:OE2	2.21	0.41
1:A:269:LYS:HB3	1:A:269:LYS:HE2	1.89	0.41
1:A:74:ASN:HA	1:A:112:ASP:HB3	2.02	0.41
1:A:88:LYS:HB3	1:A:88:LYS:NZ	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1114:TRP:HD1	1:B:1115:ARG:HD2	1.86	0.41
1:B:922:PRO:HB3	1:B:1064:LEU:O	2.21	0.41
1:D:1932:GLU:HG3	1:D:2001:PHE:CZ	2.55	0.41
1:D:2223:LEU:HA	1:D:2223:LEU:HD23	1.89	0.41
1:E:3366:LYS:HB2	1:E:3366:LYS:HE2	1.94	0.41
1:G:4273:MET:CE	1:G:4286:THR:CG2	2.99	0.41
1:G:4488:GLY:C	1:G:4489:ILE:HG12	2.41	0.41
1:E:3024:THR:HB	1:G:4596:GLU:HG2	2.03	0.41
1:G:4721:THR:HG23	1:G:4721:THR:O	2.20	0.41
1:H:4821:MET:HE3	1:H:4821:MET:CA	2.49	0.41
1:B:1104:LYS:H	1:B:1104:LYS:HG2	1.42	0.41
1:B:866:ILE:HG21	1:B:866:ILE:HD13	1.81	0.41
1:C:1273:MET:CE	1:C:1286:THR:HG21	2.49	0.41
1:D:1817:LEU:HA	1:D:1820:ALA:HB2	2.03	0.41
1:D:1819:ALA:O	1:D:1828:HIS:ND1	2.50	0.41
1:D:1875:PHE:CE1	1:D:1911:LEU:HG	2.56	0.41
1:D:2167:GLY:HA3	6:D:6414:HOH:O	2.20	0.41
1:E:3463:HIS:CE1	1:E:3470:PRO:HG2	2.56	0.41
1:E:3366:LYS:HG2	5:E:3535:ATP:C1'	2.51	0.41
1:F:3632:LEU:HA	1:F:3632:LEU:HD23	1.90	0.41
1:F:3731:VAL:HG12	1:F:3802:LEU:CB	2.42	0.41
1:H:4960:TYR:HD2	1:H:4963:ILE:HB	1.86	0.41
1:H:5089:ILE:HG22	1:H:5090:MET:N	2.35	0.41
1:H:5199:ARG:O	1:H:5202:SER:OG	2.29	0.41
1:A:215:VAL:HG21	1:A:217:LEU:HD12	2.01	0.41
1:A:461:GLN:O	1:A:464:LEU:HB2	2.21	0.41
1:B:718:ILE:CD1	1:B:810:LEU:HD22	2.51	0.41
1:C:1410:LEU:HD12	1:C:1410:LEU:HA	1.81	0.41
1:C:1628:ILE:HD13	1:C:1692:ALA:CB	2.51	0.41
1:C:1647:ALA:HB1	1:C:1648:PRO:HD2	2.02	0.41
1:C:1701:PHE:HA	1:C:1701:PHE:HD1	1.52	0.41
1:D:1855:ARG:HH22	1:D:1885:GLU:HB3	1.85	0.41
1:D:2295:VAL:HG12	1:D:2299:ARG:HG3	2.01	0.41
1:E:3228:LEU:HD12	1:E:3256:ILE:HG21	2.03	0.41
1:F:3788:GLY:HA3	1:F:3791:PHE:CE1	2.55	0.41
1:G:4248:CYS:HB2	1:G:4268:MET:HE3	1.99	0.41
1:G:4277:HIS:HE1	1:G:4405:LYS:O	2.04	0.41
1:H:4873:MET:CE	1:H:4887:ILE:CD1	2.98	0.41
1:H:5090:MET:HE3	1:H:5126:ALA:CB	2.51	0.41
1:G:4621:LYS:HG2	1:H:5210:ALA:HA	2.03	0.41
1:A:490:ASN:HA	1:A:493:MET:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1428:LEU:HA	1:C:1428:LEU:HD23	1.78	0.41
1:D:1986:GLN:O	1:D:1992:LEU:HA	2.21	0.41
1:F:4127:VAL:HA	1:F:4128:PRO:HD3	1.68	0.41
1:G:4251:GLY:C	1:G:4255:ARG:HG3	2.41	0.41
1:G:4302:ILE:HG23	1:G:4695:VAL:HA	2.03	0.41
1:G:4305:ARG:HA	1:G:4306:PRO:HD2	2.00	0.41
1:G:4275:PHE:HZ	1:G:4430:PHE:CE2	2.39	0.41
1:G:4429:LYS:HE2	1:G:4456:ILE:O	2.20	0.41
1:H:4923:ILE:C	1:H:4925:GLY:H	2.25	0.41
1:H:5193:LEU:HD21	1:H:5244:ARG:HG3	2.03	0.41
1:A:77:HIS:NE2	5:A:535:ATP:H2'	2.37	0.40
1:B:838:MET:SD	1:B:1064:LEU:HD21	2.62	0.40
1:C:1720:PHE:CZ	1:C:1722:ASN:HB3	2.56	0.40
1:D:2093:ARG:NH1	1:D:2127:THR:O	2.55	0.40
1:E:3119:ARG:O	1:E:3158:LEU:HD12	2.21	0.40
1:E:3142:THR:CG2	1:E:3144:ASP:CB	3.00	0.40
1:F:3733:LEU:HB3	1:F:3796:VAL:HG21	2.03	0.40
1:F:4093:MET:HE2	1:F:4129:VAL:HG22	2.02	0.40
1:H:4988:GLY:HA3	1:H:4991:PHE:CZ	2.55	0.40
1:H:5090:MET:CE	1:H:5126:ALA:CB	2.99	0.40
1:A:259:GLU:O	1:A:262:LYS:HG2	2.22	0.40
1:A:293:ARG:HA	1:A:296:LEU:HB3	2.03	0.40
1:A:349:ASN:HD21	1:C:1510:LYS:NZ	2.20	0.40
1:A:493:MET:CE	1:A:529:VAL:HG13	2.51	0.40
1:B:700:ASP:HA	1:B:701:PRO:HD2	1.89	0.40
1:B:851:HIS:CE1	1:B:885:ALA:HB1	2.56	0.40
1:B:845:ARG:O	1:B:878:ARG:HD3	2.21	0.40
1:C:1261:LYS:HG3	1:C:1293:ALA:HB1	2.04	0.40
1:C:1250:ILE:CG2	1:C:1286:THR:CG2	2.99	0.40
1:D:1873:MET:HG2	1:D:1887:ILE:HD11	2.02	0.40
1:E:3048:CYS:HB2	1:E:3068:MET:CE	2.37	0.40
1:E:3398:ALA:CB	1:E:3413:MET:CE	3.00	0.40
1:G:4212:ILE:HD12	1:G:4235:ASP:HB2	2.04	0.40
1:G:4377:ASP:HA	1:G:4498:ILE:CD1	2.51	0.40
1:B:934:ILE:HG23	1:B:967:GLY:CA	2.50	0.40
1:C:1300:ASP:OD2	1:C:1303:LEU:HG	2.21	0.40
1:C:1276:SER:CB	1:C:1319:ARG:NH1	2.84	0.40
1:C:1378:GLY:HA3	1:C:1498:ILE:CG1	2.49	0.40
1:C:1445:ARG:HB3	1:C:1474:GLU:OE1	2.22	0.40
1:C:1569:TYR:HB3	1:C:1572:GLU:HB2	2.03	0.40
1:D:2027:ASP:O	1:D:2030:PHE:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2188:MET:CE	1:D:2266:ARG:NH2	2.85	0.40
1:F:3756:LEU:HD12	1:F:3756:LEU:C	2.41	0.40
1:G:4276:SER:HB3	1:G:4319:ARG:HH21	1.86	0.40
1:G:4483:LEU:O	1:G:4483:LEU:HD12	2.21	0.40
1:A:206:LYS:HD2	1:A:206:LYS:HA	1.95	0.40
1:A:238:MET:CE	1:A:464:LEU:CD2	2.99	0.40
1:B:922:PRO:HG3	1:B:1065:TYR:CE2	2.55	0.40
1:B:716:PRO:HG2	1:B:843:PHE:CG	2.56	0.40
1:B:751:CYS:HB3	1:B:756:LEU:HD23	2.03	0.40
1:C:1374:TYR:HE2	1:C:1411:PRO:HG2	1.86	0.40
1:B:910:LYS:HB3	1:D:1829:MET:HG2	2.04	0.40
1:D:2041:ALA:O	1:D:2044:ILE:HG12	2.22	0.40
1:F:3928:GLN:NE2	1:H:5141:ARG:HG2	2.36	0.40
1:H:4848:CYS:SG	1:H:4868:MET:HB2	2.61	0.40
1:H:5283:GLU:HA	1:H:5286:ASP:HB2	2.04	0.40
1:A:328:GLN:HE21	1:C:1541:ARG:N	2.07	0.40
1:C:1215:GLN:CG	1:C:1239:ILE:HG23	2.51	0.40
1:C:1387:LYS:CB	1:C:1392:LEU:CD1	3.00	0.40
1:C:1677:VAL:CG1	1:C:1678:GLN:N	2.85	0.40
1:D:1873:MET:CE	1:D:1886:THR:CG2	3.00	0.40
1:D:2130:LEU:HD23	1:D:2143:GLU:HB3	2.04	0.40
1:E:3527:VAL:HA	1:E:3528:PRO:HD3	1.82	0.40
1:F:3655:ARG:CZ	1:F:3682:TYR:CE2	3.04	0.40
1:F:3675:PHE:CE1	1:F:3683:HIS:CD2	3.09	0.40
1:F:3741:ILE:HA	1:F:3756:LEU:O	2.22	0.40
1:F:3719:ARG:H	1:F:3759:ASP:HB2	1.87	0.40
1:G:4327:GLY:HA2	1:G:4404:SER:OG	2.22	0.40

All (24) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3149:GLU:OE1	1:H:4934:LYS:CE[3_655]	0.67	1.53
1:E:3149:GLU:CD	1:H:4934:LYS:NZ[3_655]	1.03	1.17
1:E:3149:GLU:CD	1:H:4934:LYS:CE[3_655]	1.23	0.97
1:D:1924:LYS:NZ	1:H:4858:GLU:OE1[1_455]	1.38	0.82
1:E:3149:GLU:OE1	1:H:4934:LYS:CD[3_655]	1.43	0.77
1:E:3081:GLU:OE1	1:H:4924:LYS:NZ[3_655]	1.49	0.71
1:E:3149:GLU:OE2	1:H:4934:LYS:NZ[3_655]	1.51	0.69
1:D:1924:LYS:CE	1:H:4858:GLU:OE1[1_455]	1.56	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3149:GLU:OE1	1:H:4934:LYS:NZ[3_655]	1.56	0.64
1:C:1387:LYS:O	1:H:4987:LYS:CB[3_645]	1.66	0.54
1:D:1948:MET:CE	1:F:3765:LYS:NZ[4_465]	1.67	0.53
1:D:1945:ASN:OD1	1:F:3816:ASP:OD2[4_465]	1.85	0.35
1:E:3149:GLU:OE2	1:H:4934:LYS:CE[3_655]	1.85	0.35
1:E:3124:LYS:C	6:H:6911:HOH:O[3_655]	1.86	0.34
1:C:1386:GLN:CB	1:H:4989:PRO:CD[3_645]	1.87	0.33
1:E:3124:LYS:O	6:H:6911:HOH:O[3_655]	1.88	0.32
1:D:1924:LYS:NZ	1:H:4858:GLU:CD[1_455]	2.00	0.20
1:C:1389:PRO:CG	1:H:4985:LYS:O[3_645]	2.02	0.18
1:E:3149:GLU:CG	1:H:4934:LYS:NZ[3_655]	2.03	0.17
1:A:277:ARG:NH1	1:G:4425:ILE:CD1[4_465]	2.07	0.13
1:A:277:ARG:CZ	1:G:4425:ILE:CD1[4_465]	2.10	0.10
1:C:1387:LYS:O	1:H:4987:LYS:CA[3_645]	2.11	0.09
1:E:3081:GLU:OE1	1:H:4924:LYS:CE[3_655]	2.17	0.03
1:C:1385:LYS:O	1:H:4989:PRO:CG[3_645]	2.19	0.01

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	517/530 (98%)	476 (92%)	36 (7%)	5 (1%)	15	15
1	B	517/530 (98%)	485 (94%)	30 (6%)	2 (0%)	34	38
1	C	517/530 (98%)	464 (90%)	42 (8%)	11 (2%)	7	4
1	D	517/530 (98%)	487 (94%)	27 (5%)	3 (1%)	25	27
1	E	517/530 (98%)	484 (94%)	26 (5%)	7 (1%)	11	9
1	F	517/530 (98%)	486 (94%)	27 (5%)	4 (1%)	19	20
1	G	517/530 (98%)	487 (94%)	27 (5%)	3 (1%)	25	27
1	H	517/530 (98%)	485 (94%)	27 (5%)	5 (1%)	15	15
All	All	4136/4240 (98%)	3854 (93%)	242 (6%)	40 (1%)	15	15

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	1337	ALA
1	C	1533	MET
1	F	3729	ALA
1	F	3789	PRO
1	G	4389	PRO
1	H	4924	LYS
1	A	221	SER
1	C	1532	SER
1	D	2058	GLY
1	E	3013	GLN
1	E	3164	CYS
1	E	3506	ASP
1	F	3730	GLU
1	A	171	SER
1	C	1320	THR
1	G	4345	ASN
1	A	327	THR
1	B	927	THR
1	C	1346	ALA
1	E	3145	ASN
1	F	3927	THR
1	A	390	HIS
1	C	1389	PRO
1	C	1527	THR
1	D	2127	THR
1	G	4458	GLY
1	H	5092	ALA
1	A	260	LYS
1	C	1371	SER
1	D	1963	ILE
1	E	3211	PRO
1	E	3327	THR
1	H	4901	PRO
1	H	5127	THR
1	H	5317	GLY
1	B	1128	PRO
1	C	1728	PRO
1	E	3258	GLY
1	C	1363	ILE
1	C	1410	LEU

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	426/434 (98%)	348 (82%)	78 (18%)	1	1
1	B	426/434 (98%)	377 (88%)	49 (12%)	5	5
1	C	426/434 (98%)	346 (81%)	80 (19%)	1	1
1	D	426/434 (98%)	379 (89%)	47 (11%)	6	5
1	E	426/434 (98%)	370 (87%)	56 (13%)	4	4
1	F	426/434 (98%)	365 (86%)	61 (14%)	3	3
1	G	426/434 (98%)	367 (86%)	59 (14%)	3	3
1	H	426/434 (98%)	384 (90%)	42 (10%)	8	7
All	All	3408/3472 (98%)	2936 (86%)	472 (14%)	3	3

All (472) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	THR
1	A	15	GLN
1	A	56	SER
1	A	60	LEU
1	A	63	MET
1	A	68	MET
1	A	73	MET
1	A	79	THR
1	A	86	THR
1	A	88	LYS
1	A	91	ARG
1	A	92	THR
1	A	96	SER
1	A	99	SER
1	A	113	THR
1	A	120	THR
1	A	130	GLU
1	A	131	VAL
1	A	133	LEU

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Mol	Chain	Res	Type
1	A	134	LYS
1	A	138	THR
1	A	145	ASN
1	A	148	MET
1	A	153	GLU
1	A	156	LEU
1	A	158	LEU
1	A	162	ASN
1	A	164	CYS
1	A	166	VAL
1	A	167	VAL
1	A	168	ASP
1	A	175	VAL
1	A	180	ILE
1	A	185	LYS
1	A	189	PRO
1	A	190	ASP
1	A	192	LEU
1	A	202	LEU
1	A	206	LYS
1	A	210	LEU
1	A	215	VAL
1	A	223	LYS
1	A	245	ARG
1	A	246	LYS
1	A	257	LEU
1	A	260	LYS
1	A	267	ILE
1	A	271	GLU
1	A	278	ARG
1	A	283	LEU
1	A	293	ARG
1	A	311	MET
1	A	330	LEU
1	A	366	LYS
1	A	375	ARG
1	A	376	MET
1	A	380	ILE
1	A	389	PHE
1	A	397	LEU
1	A	400	SER
1	A	405	THR

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Mol	Chain	Res	Type
1	A	407	LEU
1	A	411	MET
1	A	423	LEU
1	A	435	ARG
1	A	464	LEU
1	A	471	VAL
1	A	478	GLN
1	A	479	GLU
1	A	493	MET
1	A	497	LYS
1	A	499	ARG
1	A	502	PHE
1	A	508	VAL
1	A	518	SER
1	A	521	THR
1	A	522	ASN
1	A	527	VAL
1	B	615	GLN
1	B	640	THR
1	B	654	SER
1	B	660	LEU
1	B	661	LYS
1	B	673	MET
1	B	676	SER
1	B	681	GLU
1	B	702	ILE
1	B	703	LEU
1	B	719	ARG
1	B	748	MET
1	B	756	LEU
1	B	781	SER
1	B	782	LEU
1	B	785	LYS
1	B	786	GLN
1	B	787	LYS
1	B	795	GLU
1	B	798	ASN
1	B	810	LEU
1	B	822	GLU
1	B	833	GLU
1	B	839	VAL
1	B	846	LYS

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Mol	Chain	Res	Type
1	B	867	ILE
1	B	883	LEU
1	B	886	SER
1	B	917	ASN
1	B	952	LEU
1	B	966	LYS
1	B	989	PHE
1	B	1035	ARG
1	B	1039	GLN
1	B	1042	ARG
1	B	1046	ARG
1	B	1058	THR
1	B	1064	LEU
1	B	1066	ARG
1	B	1078	GLN
1	B	1086	ASP
1	B	1090	ASN
1	B	1093	MET
1	B	1099	ARG
1	B	1102	PHE
1	B	1103	LYS
1	B	1104	LYS
1	B	1107	VAL
1	B	1125	ARG
1	C	1214	THR
1	C	1227	GLU
1	C	1229	MET
1	C	1240	THR
1	C	1257	VAL
1	C	1273	MET
1	C	1279	THR
1	C	1281	GLU
1	C	1288	LYS
1	C	1292	THR
1	C	1295	GLU
1	C	1302	ILE
1	C	1305	ARG
1	C	1313	THR
1	C	1319	ARG
1	C	1323	ILE
1	C	1328	THR
1	C	1334	LYS

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Mol	Chain	Res	Type
1	C	1335	LYS
1	C	1342	THR
1	C	1348	MET
1	C	1358	LEU
1	C	1359	ASP
1	C	1363	ILE
1	C	1372	LYS
1	C	1380	ILE
1	C	1387	LYS
1	C	1390	ASP
1	C	1394	THR
1	C	1395	GLU
1	C	1404	SER
1	C	1405	LYS
1	C	1406	LYS
1	C	1410	LEU
1	C	1415	VAL
1	C	1422	GLU
1	C	1442	SER
1	C	1446	LYS
1	C	1454	ARG
1	C	1456	ILE
1	C	1457	LEU
1	C	1459	GLU
1	C	1462	LYS
1	C	1469	LYS
1	C	1472	ASN
1	C	1477	ARG
1	C	1483	LEU
1	C	1484	GLU
1	C	1486	SER
1	C	1490	MET
1	C	1493	ARG
1	C	1498	ILE
1	C	1518	ARG
1	C	1522	PRO
1	C	1529	MET
1	C	1532	SER
1	C	1538	ARG
1	C	1566	LYS
1	C	1582	ARG
1	C	1583	GLU

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Mol	Chain	Res	Type
1	C	1589	PHE
1	C	1592	LYS
1	C	1597	LEU
1	C	1599	ARG
1	C	1600	SER
1	C	1607	LEU
1	C	1633	SER
1	C	1642	ARG
1	C	1650	ILE
1	C	1664	LEU
1	C	1666	ARG
1	C	1675	ASP
1	C	1678	GLN
1	C	1679	GLU
1	C	1686	ASP
1	C	1687	LEU
1	C	1693	MET
1	C	1702	PHE
1	C	1718	SER
1	C	1723	THR
1	D	1824	THR
1	D	1829	MET
1	D	1848	CYS
1	D	1856	SER
1	D	1860	LEU
1	D	1873	MET
1	D	1887	ILE
1	D	1899	SER
1	D	1902	ILE
1	D	1919	ARG
1	D	1924	LYS
1	D	1930	GLU
1	D	1931	VAL
1	D	1938	THR
1	D	1942	THR
1	D	1945	ASN
1	D	1955	ILE
1	D	1959	ASP
1	D	1962	ASN
1	D	1966	VAL
1	D	1967	VAL
1	D	1972	LYS

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Mol	Chain	Res	Type
1	D	1985	LYS
1	D	1986	GLN
1	D	1990	ASP
1	D	2046	LYS
1	D	2059	GLU
1	D	2068	SER
1	D	2077	ARG
1	D	2099	GLU
1	D	2117	ASN
1	D	2141	ARG
1	D	2145	SER
1	D	2166	LYS
1	D	2175	ARG
1	D	2189	PHE
1	D	2199	ARG
1	D	2205	THR
1	D	2209	GLU
1	D	2246	ARG
1	D	2266	ARG
1	D	2279	GLU
1	D	2283	GLU
1	D	2293	MET
1	D	2303	LYS
1	D	2308	VAL
1	D	2318	SER
1	E	3013	GLN
1	E	3014	THR
1	E	3016	GLN
1	E	3029	MET
1	E	3034	ILE
1	E	3054	SER
1	E	3055	ARG
1	E	3056	SER
1	E	3066	SER
1	E	3080	HIS
1	E	3081	GLU
1	E	3099	SER
1	E	3102	ILE
1	E	3113	THR
1	E	3124	LYS
1	E	3131	VAL
1	E	3133	LEU

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Mol	Chain	Res	Type
1	E	3143	LEU
1	E	3145	ASN
1	E	3148	MET
1	E	3155	ILE
1	E	3156	LEU
1	E	3158	LEU
1	E	3162	ASN
1	E	3164	CYS
1	E	3165	LYS
1	E	3166	VAL
1	E	3167	VAL
1	E	3222	GLU
1	E	3246	LYS
1	E	3254	ARG
1	E	3257	LEU
1	E	3259	GLU
1	E	3265	LYS
1	E	3271	GLU
1	E	3274	GLU
1	E	3283	LEU
1	E	3286	SER
1	E	3315	ARG
1	E	3330	LEU
1	E	3336	LYS
1	E	3338	ARG
1	E	3366	LYS
1	E	3379	LEU
1	E	3382	ARG
1	E	3389	PHE
1	E	3407	LEU
1	E	3435	ARG
1	E	3442	ARG
1	E	3446	ARG
1	E	3458	THR
1	E	3466	ARG
1	E	3479	GLU
1	E	3483	GLU
1	E	3504	LYS
1	E	3526	VAL
1	F	3613	GLN
1	F	3615	GLN
1	F	3623	ASP

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Mol	Chain	Res	Type
1	F	3624	THR
1	F	3640	THR
1	F	3655	ARG
1	F	3666	SER
1	F	3673	MET
1	F	3679	THR
1	F	3687	ILE
1	F	3696	SER
1	F	3705	ARG
1	F	3713	THR
1	F	3714	LYS
1	F	3723	ILE
1	F	3726	SER
1	F	3728	THR
1	F	3731	VAL
1	F	3732	GLU
1	F	3742	THR
1	F	3743	LEU
1	F	3753	GLU
1	F	3755	ILE
1	F	3759	ASP
1	F	3762	ASN
1	F	3765	LYS
1	F	3767	VAL
1	F	3772	LYS
1	F	3782	LEU
1	F	3787	LYS
1	F	3792	LEU
1	F	3804	SER
1	F	3805	LYS
1	F	3810	LEU
1	F	3821	SER
1	F	3823	LYS
1	F	3845	ARG
1	F	3846	LYS
1	F	3856	ILE
1	F	3862	LYS
1	F	3867	ILE
1	F	3872	ASN
1	F	3878	ARG
1	F	3884	GLU
1	F	3886	SER

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Mol	Chain	Res	Type
1	F	3918	ARG
1	F	3934	ILE
1	F	3945	SER
1	F	3966	LYS
1	F	3976	MET
1	F	3989	PHE
1	F	3992	LYS
1	F	3999	ARG
1	F	4002	SER
1	F	4015	SER
1	F	4032	GLU
1	F	4066	ARG
1	F	4079	GLU
1	F	4093	MET
1	F	4107	VAL
1	F	4118	SER
1	G	4212	ILE
1	G	4213	GLN
1	G	4215	GLN
1	G	4240	THR
1	G	4255	ARG
1	G	4258	GLU
1	G	4265	LYS
1	G	4268	MET
1	G	4273	MET
1	G	4296	SER
1	G	4303	LEU
1	G	4313	THR
1	G	4319	ARG
1	G	4320	THR
1	G	4330	GLU
1	G	4338	THR
1	G	4359	ASP
1	G	4361	LYS
1	G	4367	VAL
1	G	4371	SER
1	G	4372	LYS
1	G	4375	VAL
1	G	4380	ILE
1	G	4382	LEU
1	G	4383	GLN
1	G	4386	GLN

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Mol	Chain	Res	Type
1	G	4387	LYS
1	G	4390	ASP
1	G	4392	LEU
1	G	4395	GLU
1	G	4402	LEU
1	G	4404	SER
1	G	4417	LEU
1	G	4423	LYS
1	G	4427	ASP
1	G	4442	SER
1	G	4449	ASP
1	G	4486	SER
1	G	4498	ILE
1	G	4500	ILE
1	G	4517	ASN
1	G	4545	SER
1	G	4552	LEU
1	G	4576	MET
1	G	4589	PHE
1	G	4597	LEU
1	G	4599	ARG
1	G	4600	SER
1	G	4627	LEU
1	G	4639	GLN
1	G	4656	HIS
1	G	4664	LEU
1	G	4666	ARG
1	G	4675	ASP
1	G	4693	MET
1	G	4703	LYS
1	G	4715	ARG
1	G	4718	SER
1	G	4720	PHE
1	H	4814	THR
1	H	4827	GLU
1	H	4844	THR
1	H	4855	ARG
1	H	4866	SER
1	H	4879	THR
1	H	4887	ILE
1	H	4896	SER
1	H	4899	SER

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Mol	Chain	Res	Type
1	H	4905	ARG
1	H	4922	LEU
1	H	4926	SER
1	H	4932	GLU
1	H	4934	LYS
1	H	4935	LYS
1	H	4942	THR
1	H	4948	MET
1	H	4950	LYS
1	H	4965	LYS
1	H	4972	LYS
1	H	4983	GLN
1	H	4986	GLN
1	H	4992	LEU
1	H	5002	LEU
1	H	5010	LEU
1	H	5046	LYS
1	H	5060	LYS
1	H	5067	ILE
1	H	5071	GLU
1	H	5072	ASN
1	H	5118	ARG
1	H	5182	ARG
1	H	5189	PHE
1	H	5206	ASP
1	H	5264	LEU
1	H	5278	GLN
1	H	5286	ASP
1	H	5303	LYS
1	H	5304	LYS
1	H	5308	VAL
1	H	5318	SER
1	H	5321	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (113) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	77	HIS
1	A	89	ASN
1	A	145	ASN
1	A	162	ASN

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Mol	Chain	Res	Type
1	A	198	ASN
1	A	209	ASN
1	A	263	ASN
1	A	273	HIS
1	A	328	GLN
1	A	349	ASN
1	A	377	GLN
1	A	456	HIS
1	A	457	GLN
1	A	522	ASN
1	B	643	ASN
1	B	689	ASN
1	B	745	ASN
1	B	762	ASN
1	B	783	GLN
1	B	798	ASN
1	B	826	GLN
1	B	863	ASN
1	B	928	GLN
1	B	949	ASN
1	B	977	GLN
1	B	990	HIS
1	B	1056	HIS
1	B	1063	HIS
1	B	1078	GLN
1	C	1215	GLN
1	C	1218	HIS
1	C	1243	ASN
1	C	1345	ASN
1	C	1362	ASN
1	C	1409	ASN
1	C	1426	GLN
1	C	1472	ASN
1	C	1509	GLN
1	C	1517	ASN
1	C	1528	GLN
1	C	1549	ASN
1	C	1577	GLN
1	C	1590	HIS
1	C	1656	HIS
1	C	1678	GLN
1	D	1818	HIS

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Mol	Chain	Res	Type
1	D	1889	ASN
1	D	1945	ASN
1	D	1986	GLN
1	D	1998	ASN
1	D	2063	ASN
1	D	2128	GLN
1	D	2149	ASN
1	D	2177	GLN
1	D	2190	HIS
1	D	2256	HIS
1	D	2257	GLN
1	D	2294	ASN
1	E	3043	ASN
1	E	3080	HIS
1	E	3089	ASN
1	E	3145	ASN
1	E	3162	ASN
1	E	3186	GLN
1	E	3198	ASN
1	E	3263	ASN
1	E	3328	GLN
1	E	3349	ASN
1	E	3377	GLN
1	E	3390	HIS
1	E	3457	GLN
1	E	3463	HIS
1	F	3613	GLN
1	F	3615	GLN
1	F	3618	HIS
1	F	3643	ASN
1	F	3683	HIS
1	F	3689	ASN
1	F	3786	GLN
1	F	3798	ASN
1	F	3809	ASN
1	F	3872	ASN
1	F	3873	HIS
1	F	3928	GLN
1	F	3949	ASN
1	F	3977	GLN
1	F	4063	HIS
1	G	4215	GLN

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Mol	Chain	Res	Type
1	G	4216	GLN
1	G	4218	HIS
1	G	4243	ASN
1	G	4289	ASN
1	G	4345	ASN
1	G	4383	GLN
1	G	4398	ASN
1	G	4409	ASN
1	G	4463	ASN
1	G	4528	GLN
1	G	4549	ASN
1	G	4577	GLN
1	G	4694	ASN
1	H	4843	ASN
1	H	4889	ASN
1	H	4986	GLN
1	H	5072	ASN
1	H	5128	GLN
1	H	5149	ASN
1	H	5177	GLN
1	H	5256	HIS
1	H	5257	GLN
1	H	5261	GLN
1	H	5263	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 22 are monoatomic - leaving 14 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
5	ATP	F	4135	2,4	26,33,33	1.62	4 (15%)	31,52,52	1.04	3 (9%)
5	ATP	A	535	2,4	26,33,33	1.58	7 (26%)	31,52,52	1.33	4 (12%)
3	OXL	A	533	4	0,5,5	0.00	-	0,6,6	0.00	-
3	OXL	C	1733	4	0,5,5	0.00	-	0,6,6	0.00	-
3	OXL	H	5333	4	0,5,5	0.00	-	0,6,6	0.00	-
5	ATP	D	2335	2,4	26,33,33	1.63	6 (23%)	31,52,52	1.37	5 (16%)
3	OXL	D	2333	4	0,5,5	0.00	-	0,6,6	0.00	-
5	ATP	G	4735	2,4	26,33,33	1.59	4 (15%)	31,52,52	1.32	3 (9%)
5	ATP	E	3535	2,4	26,33,33	1.58	4 (15%)	31,52,52	1.05	2 (6%)
5	ATP	C	1735	4	26,33,33	1.59	5 (19%)	31,52,52	1.69	5 (16%)
3	OXL	E	3533	4	0,5,5	0.00	-	0,6,6	0.00	-
3	OXL	B	1133	4	0,5,5	0.00	-	0,6,6	0.00	-
3	OXL	F	4133	4	0,5,5	0.00	-	0,6,6	0.00	-
3	OXL	G	4733	4	0,5,5	0.00	-	0,6,6	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ATP	F	4135	2,4	-	0/18/38/38	0/3/3/3
5	ATP	A	535	2,4	-	3/18/38/38	0/3/3/3
3	OXL	A	533	4	-	0/0/4/4	-
3	OXL	C	1733	4	-	0/0/4/4	-
3	OXL	H	5333	4	-	0/0/4/4	-
5	ATP	D	2335	2,4	-	2/18/38/38	0/3/3/3
3	OXL	D	2333	4	-	0/0/4/4	-
5	ATP	G	4735	2,4	-	3/18/38/38	0/3/3/3
5	ATP	E	3535	2,4	-	3/18/38/38	0/3/3/3
5	ATP	C	1735	4	-	2/18/38/38	0/3/3/3
3	OXL	E	3533	4	-	0/0/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OXL	B	1133	4	-	0/0/4/4	-
3	OXL	F	4133	4	-	0/0/4/4	-
3	OXL	G	4733	4	-	0/0/4/4	-

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	3535	ATP	PG-O3G	-4.88	1.36	1.54
5	D	2335	ATP	PG-O3G	-4.80	1.36	1.54
5	C	1735	ATP	PG-O3G	-4.14	1.38	1.54
5	G	4735	ATP	PG-O3G	-4.06	1.39	1.54
5	F	4135	ATP	C2-N1	4.02	1.41	1.33
5	A	535	ATP	PG-O3G	-3.92	1.39	1.54
5	F	4135	ATP	PA-O5'	3.86	1.74	1.59
5	G	4735	ATP	O4'-C1'	-3.45	1.36	1.41
5	D	2335	ATP	C2-N1	3.22	1.39	1.33
5	F	4135	ATP	PG-O3G	-3.18	1.42	1.54
5	C	1735	ATP	PG-O1G	-3.05	1.40	1.50
5	A	535	ATP	PG-O2G	-2.85	1.43	1.54
5	C	1735	ATP	PG-O2G	-2.85	1.43	1.54
5	A	535	ATP	C2-N1	2.81	1.39	1.33
5	C	1735	ATP	O4'-C1'	-2.75	1.37	1.41
5	D	2335	ATP	PA-O5'	2.72	1.70	1.59
5	E	3535	ATP	PG-O2G	-2.72	1.44	1.54
5	C	1735	ATP	PA-O5'	2.65	1.70	1.59
5	A	535	ATP	C8-N7	2.58	1.39	1.34
5	D	2335	ATP	PG-O2G	-2.53	1.45	1.54
5	G	4735	ATP	C2'-C1'	-2.47	1.50	1.53
5	D	2335	ATP	PG-O1G	-2.43	1.42	1.50
5	E	3535	ATP	PA-O5'	2.39	1.69	1.59
5	A	535	ATP	PA-O5'	2.36	1.68	1.59
5	E	3535	ATP	C2-N1	2.31	1.38	1.33
5	A	535	ATP	PG-O1G	-2.21	1.43	1.50
5	A	535	ATP	O4'-C1'	-2.13	1.38	1.41
5	G	4735	ATP	PA-O2A	-2.11	1.45	1.55
5	D	2335	ATP	C4-N3	2.04	1.38	1.35
5	F	4135	ATP	C6-N6	2.02	1.41	1.34

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1735	ATP	C5-C6-N6	5.59	128.85	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	4735	ATP	C5-C6-N6	5.13	128.15	120.35
5	D	2335	ATP	O2G-PG-O1G	4.39	127.86	110.68
5	A	535	ATP	O2G-PG-O1G	3.73	125.28	110.68
5	C	1735	ATP	O2G-PG-O1G	3.66	125.02	110.68
5	D	2335	ATP	O3G-PG-O3B	-3.36	93.36	104.64
5	A	535	ATP	O3G-PG-O3B	-3.05	94.42	104.64
5	C	1735	ATP	O3G-PG-O3B	-2.91	94.87	104.64
5	E	3535	ATP	C5-C6-N6	2.87	124.71	120.35
5	A	535	ATP	C5-C6-N6	2.64	124.36	120.35
5	F	4135	ATP	N6-C6-N1	2.43	123.63	118.57
5	C	1735	ATP	N6-C6-N1	-2.40	113.58	118.57
5	G	4735	ATP	O3G-PG-O3B	2.30	112.35	104.64
5	F	4135	ATP	C5-C6-N1	-2.28	115.18	120.35
5	D	2335	ATP	O2G-PG-O3B	-2.28	96.99	104.64
5	D	2335	ATP	C5-C6-N6	2.27	123.80	120.35
5	A	535	ATP	C5-C6-N1	-2.23	115.30	120.35
5	G	4735	ATP	C1'-N9-C4	-2.21	122.75	126.64
5	D	2335	ATP	C2'-C3'-C4'	-2.17	98.42	102.64
5	C	1735	ATP	O3'-C3'-C2'	2.13	118.71	111.82
5	F	4135	ATP	O3G-PG-O3B	2.08	111.62	104.64
5	E	3535	ATP	O3G-PG-O3B	2.01	111.38	104.64

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	3535	ATP	PB-O3B-PG-O3G
5	D	2335	ATP	PB-O3B-PG-O3G
5	A	535	ATP	PB-O3A-PA-O1A
5	E	3535	ATP	PB-O3A-PA-O1A
5	A	535	ATP	PG-O3B-PB-O1B
5	G	4735	ATP	PA-O3A-PB-O1B
5	C	1735	ATP	PA-O3A-PB-O2B
5	E	3535	ATP	PA-O3A-PB-O1B
5	D	2335	ATP	PB-O3B-PG-O2G
5	G	4735	ATP	PB-O3B-PG-O2G
5	C	1735	ATP	PB-O3A-PA-O2A
5	A	535	ATP	PG-O3B-PB-O2B
5	G	4735	ATP	PA-O3A-PB-O2B

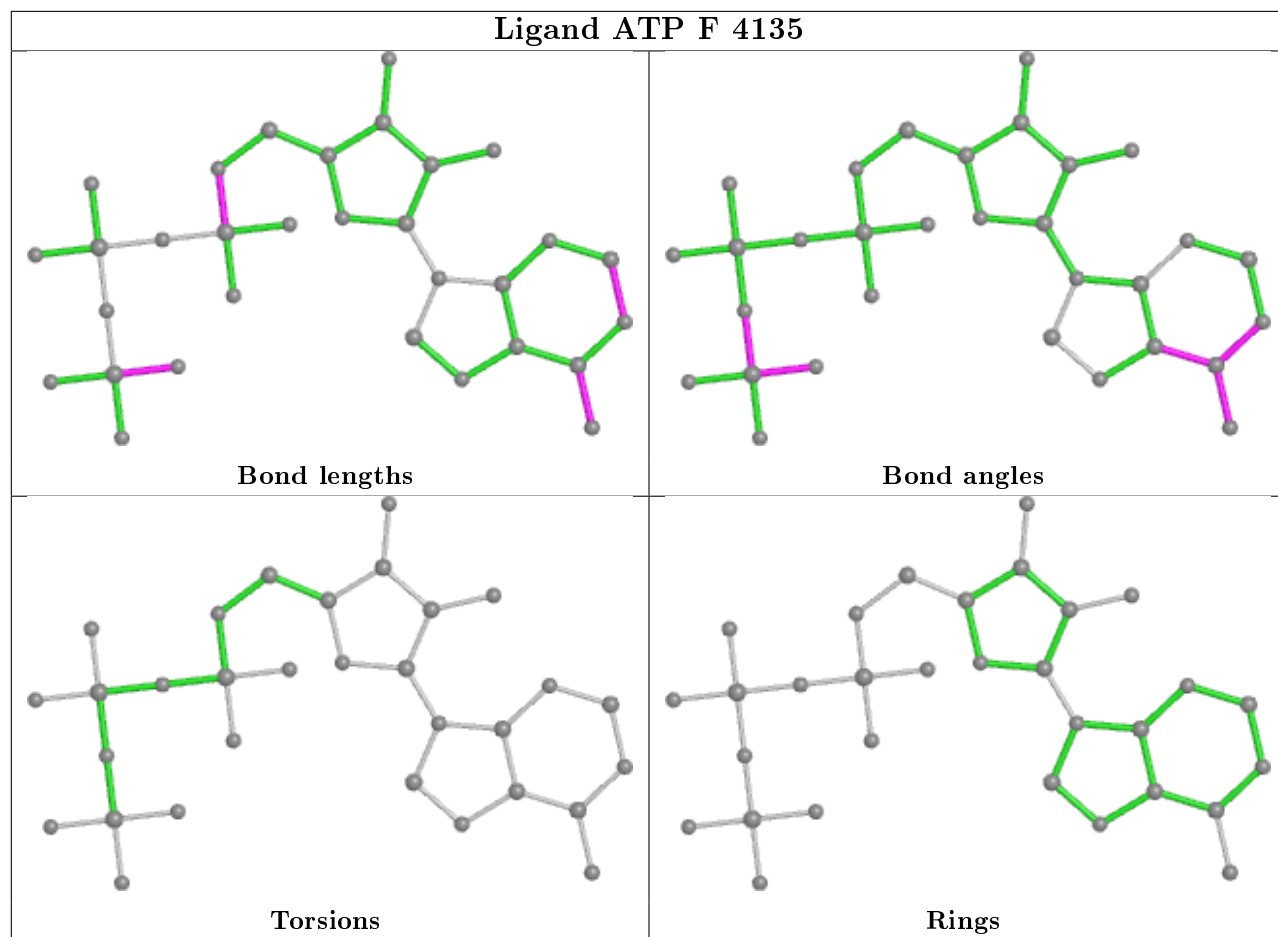
There are no ring outliers.

11 monomers are involved in 21 short contacts:

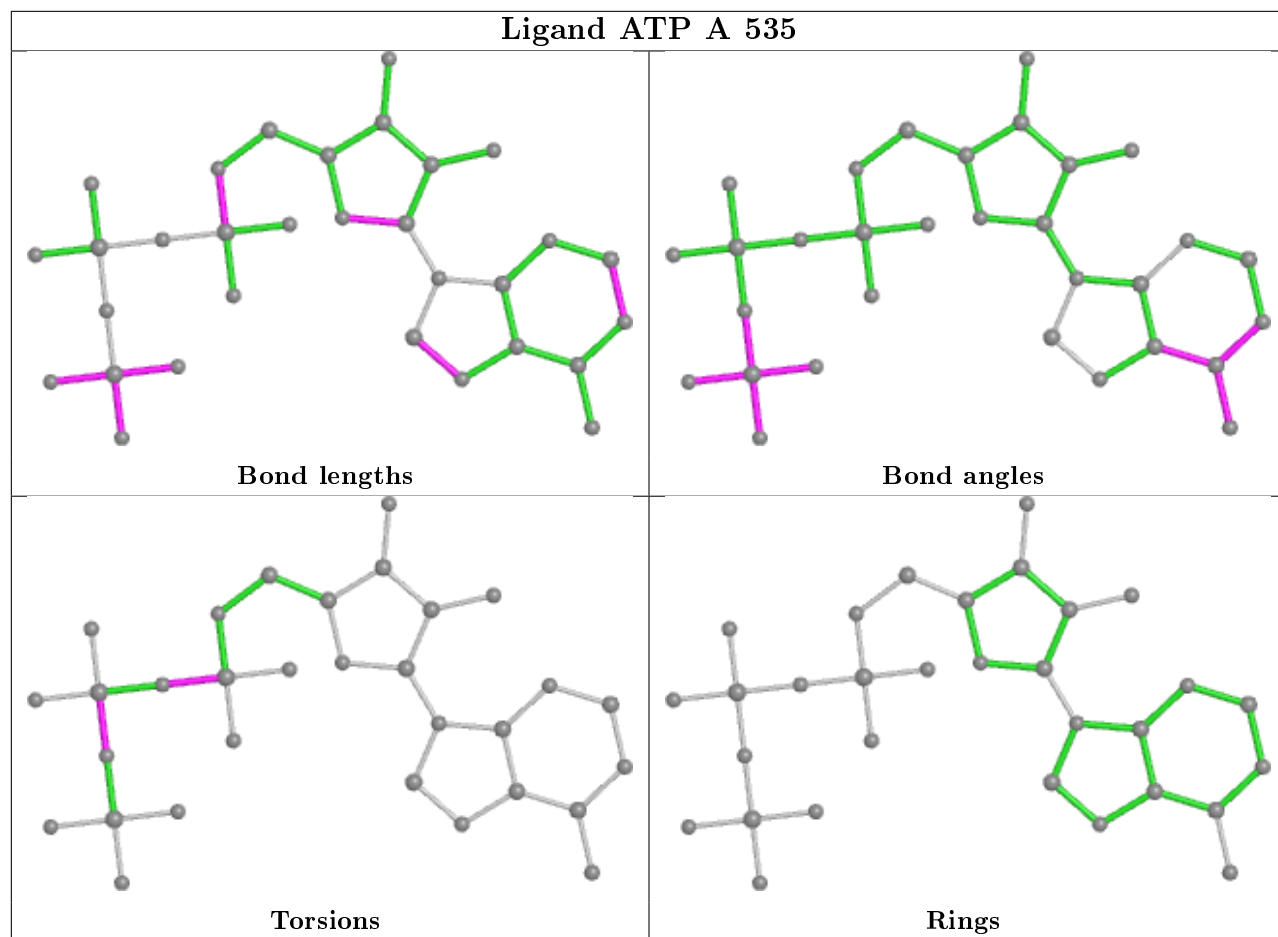


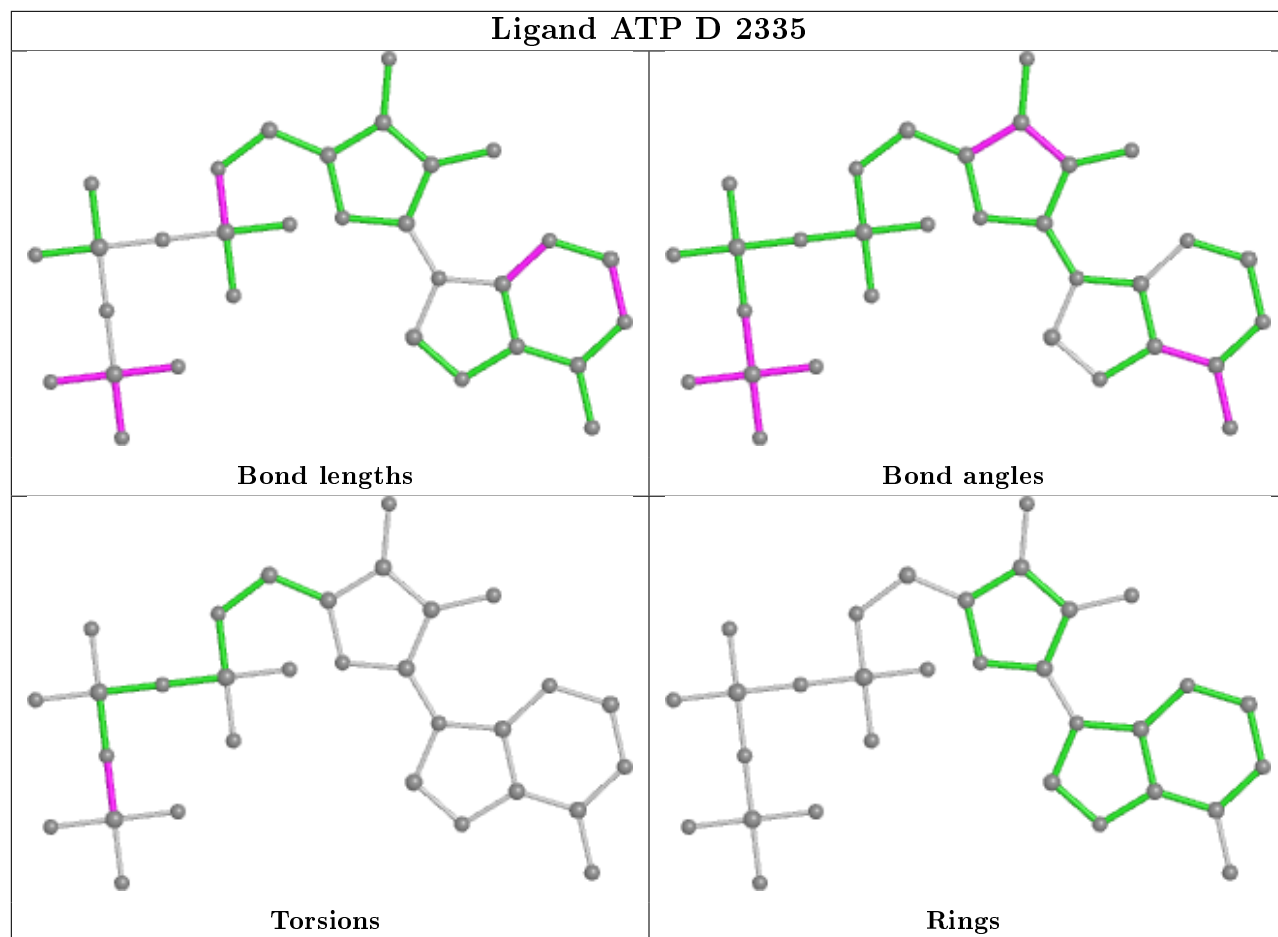
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	535	ATP	4	0
3	A	533	OXL	2	0
3	C	1733	OXL	1	0
3	H	5333	OXL	1	0
5	D	2335	ATP	1	0
3	D	2333	OXL	1	0
5	E	3535	ATP	2	0
5	C	1735	ATP	4	0
3	E	3533	OXL	1	0
3	F	4133	OXL	2	0
3	G	4733	OXL	2	0

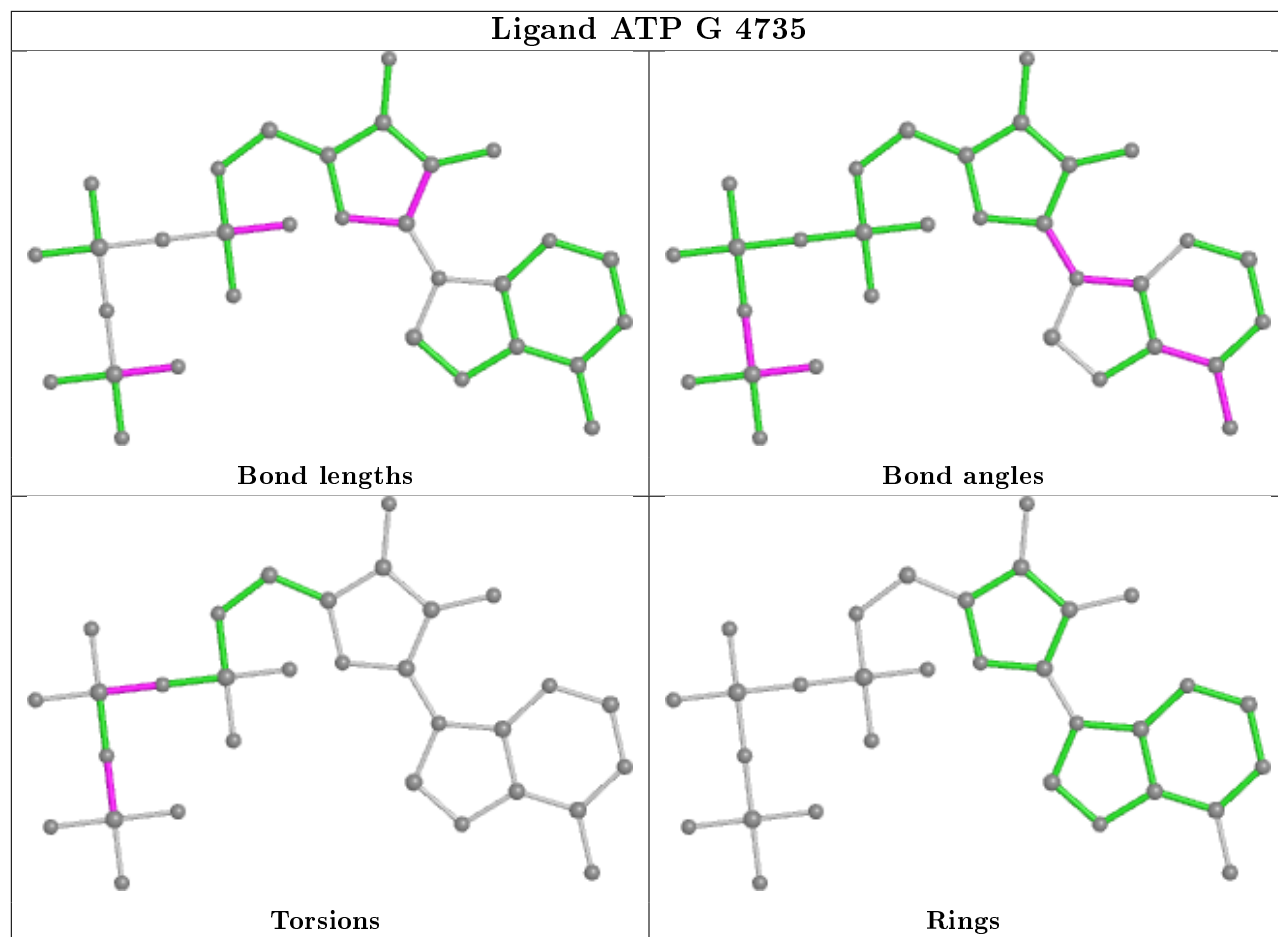
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

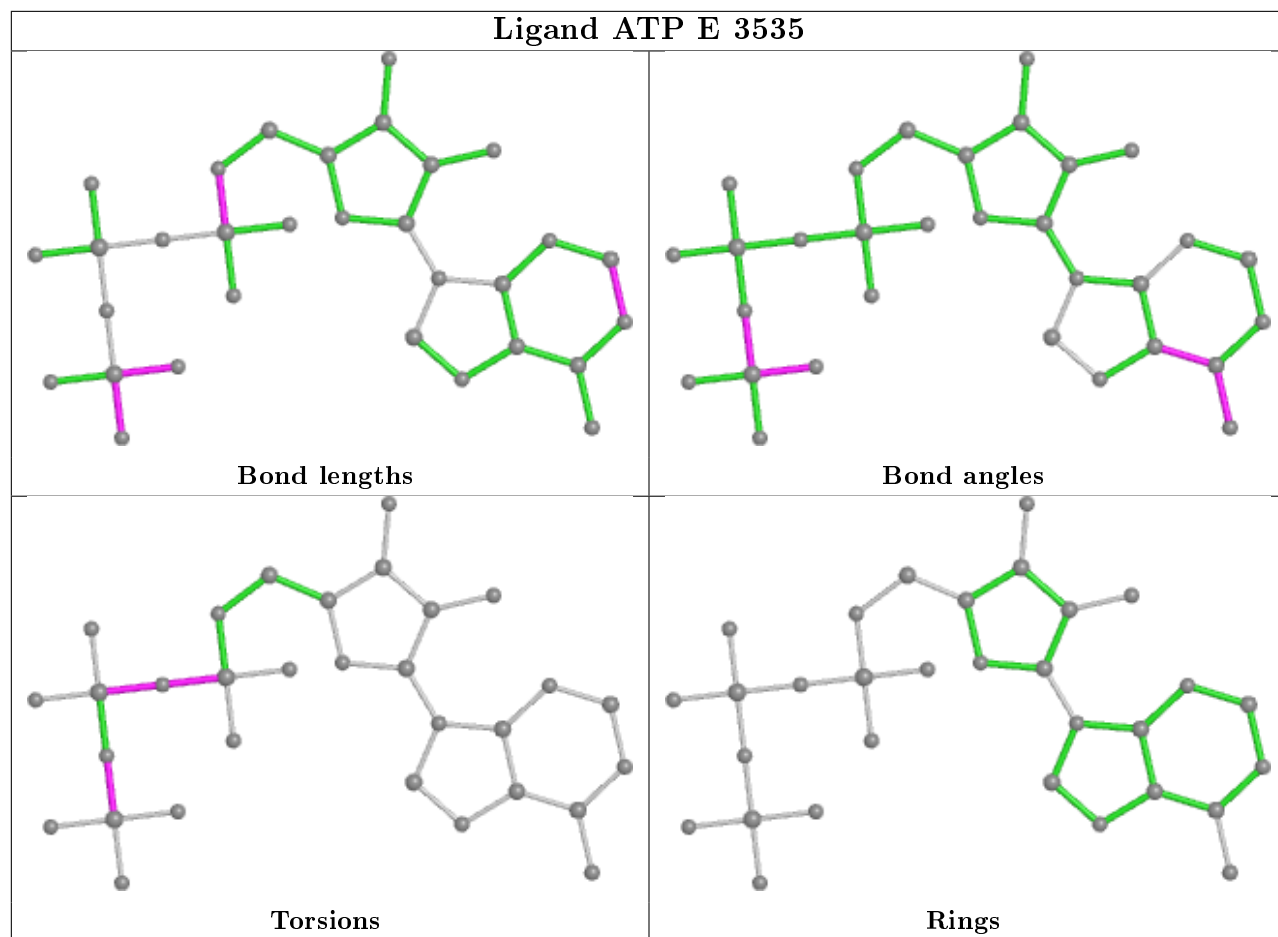


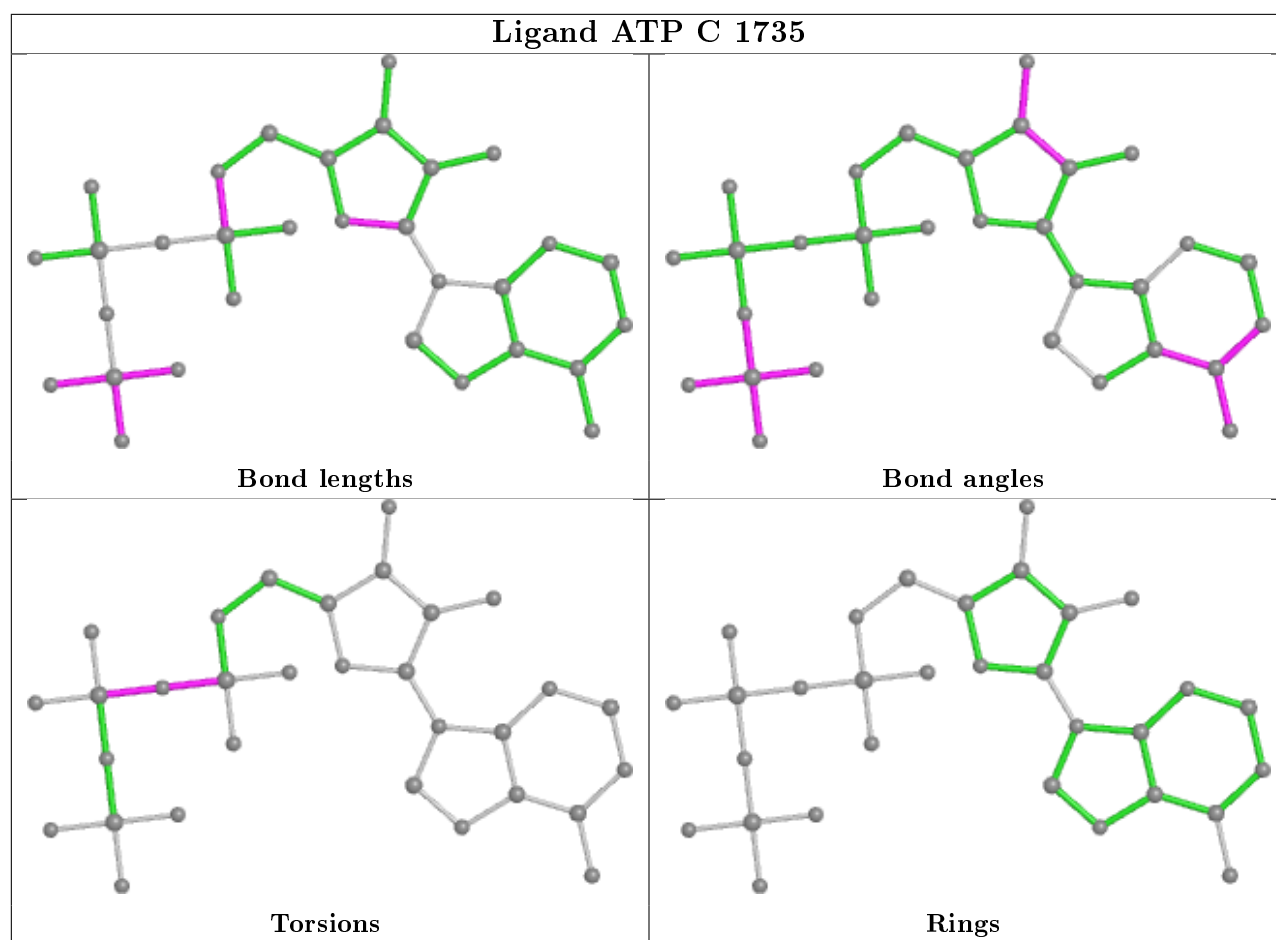
## Ligand ATP A 535











## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	241:ALA	C	242:SER	N	1.14

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.